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Chapter 1: Key Features of Quantum Mechanics

Quantum mechanics is now almost one-hundred years old, but we are still discovering some of its surprising features and it remains the subject of much investigation and speculation. The framework of quantum mechanics is a rich and elegant extension of the framework of classical physics. It is also counterintuitive and almost paradoxical.

Quantum physics has replaced classical physics as the correct fundamental description of our physical universe. It is used routinely to describe most phenomena that occur at short distances. Quantum physics is the result of applying the framework of quantum mechanics to different physical phenomena. We thus have Quantum Electrodynamics, when quantum mechanics is applied to electromagnetism, Quantum Optics, when it is applied to light and optical devices, or Quantum Gravity, when it is applied to gravitation. Quantum mechanics indeed provides a remarkably coherent and elegant framework. The era of quantum physics begins in 1925, with the discoveries of Schrödinger and Heisenberg. The seeds for these discoveries were planted by Planck, Einstein, Bohr, de Broglie, and others. It is a tribute to human imagination that we have been able to discover the counterintuitive and abstract set of rules that define quantum mechanics. Here we aim to explain and provide some perspective on the main features of this framework.

We will begin by discussing the property of linearity, which quantum mechanics shares with electromagnetic theory. This property tells us what kind of theory quantum mechanics is and why, it could be argued, it is simpler than classical mechanics. We then turn to photons, the particles of light. We use photons and polarizers to explain why quantum physics is not deterministic and, in contrast with classical physics, the results of some experiments cannot be predicted. Quantum mechanics is a framework in which we can only predict the *probabilities* for the various outcomes of any given experiment. Our next subject is quantum superpositions, in which a quantum object somehow manages to exist simultaneously in two mutually incompatible states. A quantum light-bulb, for example, could be in a state in which it is both on and off at the same time!

1 Linearity of the equations of motion

In physics a theory is usually described by a set of equations for some quantities called the **dynamical variables** of the theory. After writing a theory, the most important task is finding solutions of the equations. A solution of the equations describes a possible reality, according to the theory. Because an expanding universe is a solution of Albert Einstein's gravitational equations, for example, it follows that an expanding universe is possible, according to this theory. A single theory may have many solutions, each describing a possible reality.

There are linear theories and nonlinear theories. Nonlinear theories are more complex than linear theories. In a linear theory a remarkable fact takes place: if you have two solutions you obtain a third solution of the theory simply by adding the two solutions. An example of a beautiful linear theory is Maxwell's theory of electromagnetism, a theory that governs the behavior of electric and magnetic fields. A field, as you probably know, is a quantity whose values may depend on position and on time. A simple solution of this theory describes an electromagnetic wave propagating in a given direction. Another simple solution could describe an electromagnetic wave propagating in a

different direction. Because the theory is linear, having the two waves propagating simultaneously, each in its own direction and without affecting each other, is a new and consistent solution. The sum is a solution in the sense that the electric field in the new solution is the sum of the electric field in the first solution plus the electric field in the second solution. The same goes for the magnetic field: the magnetic field in the new solution is the sum of the magnetic field in the first solution plus the magnetic field in the second solution. In fact you can add any number of solutions to still find a solution. Even if this sounds esoteric, you are totally familiar with it. The air around you is full of electromagnetic waves, each one propagating oblivious to the other ones. There are the waves of thousands of cell phones, the waves carrying hundreds of wireless internet messages, the waves from a plethora of radio-stations, TV stations, and many, many more. Today, a single transatlantic cable can carry simultaneously millions of telephone calls, together with huge amounts video and internet data. All of that courtesy of linearity.

More concretely, we say that Maxwell's equations are **linear** equations. A solution of Maxwell's equation is described by an electric field $\mathbf{E}$ a magnetic field $\mathbf{B}$, a charge density ρ and a current density $\mathbf{J}$, all collectively denoted as $(\mathbf{E},\, \mathbf{B}\,, \rho\,,\, \mathbf{J})$. This collection of fields and sources satisfy Maxwell's equations. Linearity implies that if $(\mathbf{E},\, \mathbf{B}\,, \rho\,,\, \mathbf{J})$ is a solution so is $(\alpha\mathbf{E},\, \alpha\mathbf{B}\,, \alpha\rho\,,\, \alpha\mathbf{J})$, where all fields and sources have been multiplied by the constant α. Given two solutions

$$(\mathbf{E}_1, \mathbf{B}_1, \rho_1, \mathbf{J}_1)\,, \quad \text{and} \quad (\mathbf{E}_2, \mathbf{B}_2, \rho_2, \mathbf{J}_2)\,, \tag{1.1}$$

linearity also implies that we can obtain a new solution by adding them

$$(\mathbf{E}_1 + \mathbf{E}_2\,,\ \mathbf{B}_1 + \mathbf{B}_2\,,\ \rho_1 + \rho_2\,,\ \mathbf{J}_1 + \mathbf{J}_2)\,. \tag{1.2}$$

The new solution may be called the superposition of the two original solutions.

It is not hard to explain what is, in general, a linear equation or a linear set of equations. Consider the equation

$$L\,u \ = \ 0\,, \tag{1.3}$$

where, schematically, u denotes the unknown. The unknown may be a number, or a function of time, a function of space, a function of time and space, essentially anything unknown! In fact, u could represent a collection of unknowns, in which case we would replace u above by $u_1, u_2, \ldots$. The symbol L denotes a **linear operator**, an object that satisfies the following two properties

$$L(u_1 + u_2) \ = \ Lu_1 + Lu_2\,, \qquad L(a\,u) \ = \ aLu\,, \tag{1.4}$$

where a is a number. Note that these conditions imply that

$$L(\alpha u_1 + \beta u_2) \ = \ \alpha L u_1 + \beta L u_2\,, \tag{1.5}$$

showing that if u_1 is a solution ($Lu_1 = 0$) and u_2 is a solution ($Lu_2 = 0$) then $\alpha u_1 + \beta u_2$ is also a solution. We call $\alpha u_1 + \beta u_2$ the **general superposition** of the solutions u_1 and u_2. An example may help. Consider the equation

$$\frac{du}{dt} + \frac{1}{\tau}\,u \ = \ 0\,, \tag{1.6}$$

where τ is a constant with units of time. This is, in fact, a linear differential equation, and takes the form $L\,u = 0$ if we define

$$L\,u \ \equiv \ \frac{du}{dt} + \frac{1}{\tau}u \tag{1.7}$$

Exercise 1. Verify that (1.7) satisfies the conditions for a linear operator.

Einstein's theory of general relativity is a nonlinear theory whose dynamical variable is a gravitational field, the field that describes, for example, how planets move around a star. Being a nonlinear theory, you simply cannot add the gravitational fields of different solutions to find a new solution. This makes Einstein's theory rather complicated, by all accounts much more complicated than Maxwell theory. In fact, classical mechanics, as invented mostly by Isaac Newton, is also a nonlinear theory! In classical mechanics the dynamical variables are positions and velocities of particles, acted by forces. There is no general way to use two solutions to build a third.

Indeed, consider the equation of motion for a particle on a line under the influence of a time-independent potential $V(x)$, which is in general an arbitrary function of x. The dynamical variable in this problem is $x(t)$, the position as a function of time. Letting V' denote the derivative of V with respect to its argument, Newton's second law takes the form

$$m\,\frac{d^2x(t)}{dt^2} \;=\; -V'(x(t))\,. \tag{1.8}$$

The left-hand side is the mass times acceleration and the right hand side is the force experienced by the particle in the potential. It is probably worth to emphasize that the right hand side is the function $V'(x)$ evaluated for x set equal to $x(t)$:

$$V'(x(t)) \;\equiv \frac{\partial V(x)}{\partial x}\Big|_{x=x(t)}\,. \tag{1.9}$$

While we could have used here an ordinary derivative, we wrote a partial derivative as is commonly done for the general case of time dependent potentials. The reason equation (1.8) is not a linear equation is that the function $V'(x)$ is not linear. In general, for arbitrary functions u and v we expect

$$V'(au) \neq \; aV'(u)\,, \quad \text{and} \quad V'(u+v) \neq V'(u) + V(v)\,. \tag{1.10}$$

As a result given a solution $x(t)$, the scaled solution $\alpha x(t)$ is not expected to be a solution. Given two solutions $x_1(t)$ and $x_2(t)$ then $x_1(t) + x_2(t)$ is not guaranteed to be a solution either.

Exercise. What is the most general potential $V(x)$ for which the equation of motion for $x(t)$ is linear?

Quantum mechanics is a linear theory. The signature equation in this theory, the so-called Schrödinger equation is a linear equation for a quantity called the **wavefunction** and it determines its time evolution. The wavefunction is the dynamical variable in quantum mechanics but, curiously, its physical interpretation was not clear to Erwin Schrödinger when he wrote the equation in 1925. It was Max Born, who months later suggested that the wavefunction encodes probabilities. This was the correct physical interpretation, but it was thoroughly disliked by many, including Schrödinger, who remained unhappy about it for the rest of his life. The linearity of quantum mechanics implies a profound simplicity. In some sense quantum mechanics is simpler than classical mechanics. In quantum mechanics solutions can be added to form new solutions.

The wavefunction Ψ depends on time and may also depend on space. The Schrödinger equation (SE) is a partial differential equation that takes the form

$$i\hbar\,\frac{\partial \Psi}{\partial t} = \hat{H}\Psi\,, \tag{1.11}$$

where the Hamiltonian (or energy operator) $\hat{H}$ is a linear operator that can act on wavefunctions:

$$\hat{H}(a\Psi) \;=\; a\,\hat{H}\,\Psi\,, \qquad \hat{H}(\Psi_1+\Psi_2) \;=\; \hat{H}(\Psi_1)+\hat{H}(\Psi_2)\,, \tag{1.12}$$

with a a constant that in fact need not be real; it can be a complex number. Of course, $\hat{H}$ itself does not depend on the wavefunction! To check that the Schrödinger equation is linear we cast it in the form $L\Psi = 0$ with L defined as

$$L\Psi \;\equiv\; i\hbar\frac{\partial\Psi}{\partial t} - \hat{H}\Psi \tag{1.13}$$

It is now a simple matter to verify that L is a linear operator. Physically this means that if Ψ_1 and Ψ_2 are solutions to the Schrödinger equation, then so is the superposition $\alpha\Psi_1 + \beta\Psi_2$, where α and β are both complex numbers, i.e. $(\alpha, \beta \in \mathbb{C})$

2 Complex Numbers are Essential

Quantum mechanics is the first physics theory that truly makes use of *complex* numbers. The numbers most of us use for daily life (integers, fractions, decimals) are *real* numbers. The set of complex numbers is denoted by $\mathbb{C}$ and the set of real numbers is denoted by $\mathbb{R}$. Complex numbers appear when we combine real numbers with the imaginary unit i, defined to be equal to the square root of minus one: $i \equiv \sqrt{-1}$. Being the square root of minus one, it means that i squared must give minus one: $i^2 = -1$. Complex numbers are fundamental in mathematics. An equation like $x^2 = -4$, for an unknown x cannot be solved if x has to be real. No real number squared gives you minus one. But if we allow for complex numbers, we have the solutions $x = \pm 2i$. Mathematicians have shown that all polynomial equations can be solved in terms of complex numbers.

A complex number z, in all generality, is a number of the form

$$z \;=\; a + ib \;\in\; \mathbb{C}\,, \quad a, b \in \mathbb{R}\,. \tag{2.1}$$

Here a and b are real numbers, and ib denotes the product of i with b. The number a is called the real part of z and b is called the imaginary part of z:

$$\mathrm{Re}\, z = a\,, \qquad \mathrm{Im}\, z = b\,. \tag{2.2}$$

The complex conjugate z^* of z is defined by

$$z^* \;=\; a - ib\,. \tag{2.3}$$

You can quickly verify that a complex number z is real if $z^* = z$ and it is purely imaginary if $z^* = -z$. For any complex number $z = a+ib$ one can define the *norm* $|z|$ of the complex number to be a *positive, real* number given by

$$|z| = \sqrt{a^2 + b^2}\,. \tag{2.4}$$

You can quickly check that

$$|z|^2 = zz^*\,, \tag{2.5}$$

where $z^* \equiv a - ib$ is called the complex conjugate of $z = a + ib$. Complex numbers are represented as vectors in a two dimensional "complex plane". The real part of the complex number is the x component of the vector and the imaginary part of the complex number is the y component. If you consider the unit length vector in the complex plane making an angle θ with the x axis has x component $\cos\theta$ and

y component $\sin\theta$. The vector is therefore the complex number $\cos\theta + i\sin\theta$. Euler's identity relates this to the exponential of $i\theta$:

$$e^{i\theta} \;=\; \cos\theta + i\sin\theta\,. \tag{2.6}$$

A complex number of the form $e^{i\chi}$, with χ real is called a *pure phase*.

While complex numbers are sometimes useful in classical mechanics or Maxwell theory, they are not strictly needed. None of the dynamical variables, which correspond to measurable quantities, is a complex number. In fact, complex numbers can't be measured at all: all measurements in physics result in real numbers. In quantum mechanics, however, complex numbers are fundamental. The Schrödinger equation involves complex numbers. Even more, the wavefunction, the dynamical variable of quantum mechanics it itself a complex number:

$$\Psi \in \mathbb{C}\,. \tag{2.7}$$

Since complex numbers cannot be measured the relation between the wavefunction and a measurable quantity must be somewhat indirect. Born's idea to identify probabilities, which are always positive real numbers, with the square of the norm of the wavefuntion was very natural. If we write the wavefunction of our quantum system as Ψ, the probabilities for possible events are computed from $|\Psi|^2$. The mathematical framework required to express the laws of quantum mechanics consists of complex vector spaces. In any vector space we have objects called vectors that can be added together. In a complex vector space a vector multiplied by a complex number is still a vector. As we will see in our study of quantum mechanics it is many times useful to think of the wavefunction Ψ as a vector in some complex vector space.

3 Loss of Determinism

Maxwell's crowning achievement was the realization that his equations of electromagnetism allowed for the existence of propagating waves. In particular, in 1865 he conjectured that light was an electromagnetic wave, a propagating fluctuation of electric and magnetic fields. He was proven right in subsequent experiments. Towards the end of the nineteenth century physicists were convinced that light was a wave. The certainty, however, did not last too long. Experiments on blackbody radiation and on the photo-emission of electrons suggested that the behavior of light had to be more complicated than that of a simple wave. Max Planck and Albert Einstein were the most prominent contributors to the resolution of the puzzles raised by those experiments.

In order to explain the features of the photoelectric effect, Einstein postulated (1905) that in a light beam the energy comes in quanta – the beam is composed of packets of energy. Einstein essentially implied that light was made up of particles, each carrying a fixed amount of energy. He himself found this idea disturbing, convinced like most other contemporaries that, as Maxwell had shown, light was a wave. He anticipated that a physical entity, like light, that could behave both as a particle and as a wave could bring about the demise of classical physics and would require a completely new physical theory. He was in fact right. Though he never quite liked quantum mechanics, his ideas about particles of light, later given the name *photons*, helped construct this theory.

It took physicists until 1925 to accept that light could behave like a particle. The experiments of Arthur Compton (1923) eventually convinced most skeptics. Nowadays, particles of light, or photons, are routinely manipulated in laboratories around the world. Even if mysterious, we have grown accustomed to them. Each photon of visible light carries very little energy – a small laser pulse can

contain many billions of photons. Our eye, however, is a very good photon detector: in total darkness, we are able to see light when as little as ten photons hit upon our retina. When we say that light behaves like a particle we mean a quantum mechanical particle: a packet of energy and momentum that is not composed of smaller packets. We *do not* mean a classical point particle or Newtonian corpuscle, which is a zero-size object with definite position and velocity.

As it turns out, the energy of a photon depends only on the color of the light. As Einstein discovered the energy E and frequency ν for a photon are related by

$$E = h\nu \tag{3.1}$$

The frequency of a photon determines the wavelength λ of the light through the relation $\nu\lambda = c$, where c is the speed of light. All green photons, for example, have the same energy. To increase the energy in a light beam while keeping the same color, one simply needs more photons.

As we now explain, the existence of photons implies that Quantum Mechanics is not deterministic. By this we mean that the result of an experiment cannot be determined, as it would in classical physics, by the conditions that are under the control of the experimenter.

Consider a polarizer whose preferential direction is aligned along the $\hat{\mathbf{x}}$ direction, as shown in Figure 1. Light that is linearly polarized along the $\hat{\mathbf{x}}$ direction namely, light whose electric field points in this direction, goes through the polarizer. If the incident light polarization is orthogonal to the $\hat{\mathbf{x}}$ direction the light will not go through at all. Thus light linearly polarized in the $\hat{\mathbf{y}}$ direction will be totally absorbed by the polarizer. Now consider light polarized along a direction forming an angle α with the x-axis, as shown in Figure 2. What happens?

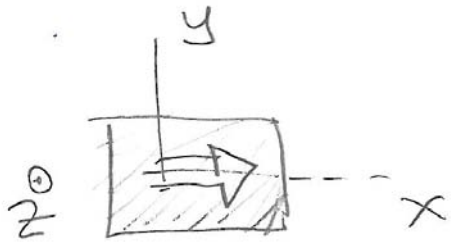

Figure 1: A polarizer that transmits light linearly polarized along the $\hat{\mathbf{x}}$ direction.

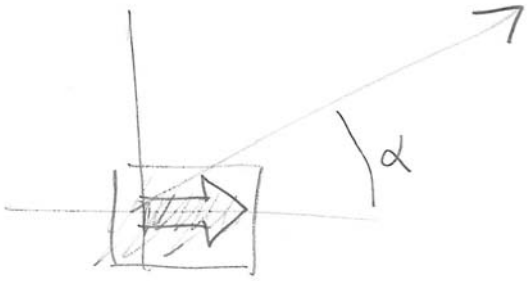

Figure 2: Light linearly polarized along the direction at an angle α hitting the polarizer.

Thinking of the light as a propagating wave, the incident electric field $\mathbf{E}_\alpha$ makes an angle α with the x-axis and therefore takes the form

$$\mathbf{E}_\alpha \;=\; E_0 \cos\alpha\; \hat{\mathbf{x}} + E_0 \sin\alpha\; \hat{\mathbf{y}}\,. \tag{3.2}$$

This is an electric field of magnitude E_0. In here we are ignoring the time and space dependence of the wave; they are not relevant to our discussion. When this electric field hits the polarizer, the component along $\hat{\mathbf{x}}$ goes through and the component along $\hat{\mathbf{y}}$ is absorbed. Thus

$$\text{Beyond the polarizer:} \qquad \mathbf{E} = E_0 \cos\alpha \; \hat{\mathbf{x}} \,. \tag{3.3}$$

You probably recall that the energy in an electromagnetic wave is proportional to the square of the magnitude of the electric field. This means that the fraction of the beam's energy that goes through the polarizer is $(\cos\alpha)^2$. It is also well known that the light emerging from the polarizer has the *same frequency* as the incident light.

So far so good. But now, let us try to understand this result by thinking about the photons that make up the incident light. The premise here is that all photons in the incident beam are identical. Moreover the photons do not interact with each other. We could even imagine sending the whole energy of the incident light beam one photon at a time. Since all the light that emerges from the polarizer has the same frequency as the incident light, and thus the same frequency, we must conclude that each individual photon either goes through or is absorbed. If a fraction of a photon went through it would be a photon of lower energy and thus lower frequency, which is something that does not happen.

But now we have a problem. As we know from the wave analysis, roughly a fraction $(\cos\alpha)^2$ of the photons must go through, since that is the fraction of the energy that is transmitted. Consequently a fraction $1-(\cos\alpha)^2$ of the photons must be absorbed. But if all the photons are identical, why is it that what happens to one photon does not happen to all of them?

The answer in quantum mechanics is that there is indeed a loss of determinism. No one can predict if a photon will go through or will get absorbed. The best anyone can do is to predict probabilities. In this case there would be a probability $(\cos\alpha)^2$ of going through and a probability $1-(\cos\alpha)^2$ of failing to go through.

Two escape routes suggest themselves. Perhaps the polarizer is not really a homogeneous object and depending exactly on where the photon his it either gets absorbed or goes through. Experiments show this is not the case. A more intriguing possibility was suggested by Einstein and others. A possible way out, they claimed, was the existence of *hidden variables.* The photons, while apparently identical, would have other *hidden* properties, not currently understood, that would determine with certainty which photon goes through and which photon gets absorbed. Hidden variable theories would seem to be untestable, but surprisingly they can be tested. Through the work of John Bell and others, physicists have devised clever experiments that rule out most versions of hidden variable theories. No one has figured out how to restore determinism to quantum mechanics. It seems to be an impossible task.

When we try to describe photons quantum mechanically we could use wavefunctions, or equivalently the language of states. A photon polarized along the $\hat{\mathbf{x}}$ direction is not represented using an electric field, but rather we just give a name for its *state*:

$$\big|\text{photon}; x\big\rangle \,. \tag{3.4}$$

We will learn the rules needed to manipulate such objects, but for the time being you could think of it like a vector in some space yet to be defined. Another state of a photon, or vector is

$$\big|\text{photon}; y\big\rangle \,, \tag{3.5}$$

representing a photon polarized along $\hat{\mathbf{y}}$. These states are the wavefunctions that represent the photon. We now claim that the photons in the beam that is polarized along the direction α are in a state $\big|\text{photon}; \alpha\big\rangle$ that can be written as a superposition of the above two states:

$$\big|\text{photon}; \alpha\big\rangle \;=\; \cos\alpha \,\big|\text{photon}; x\big\rangle + \sin\alpha \,\big|\text{photon}; y\big\rangle \,. \tag{3.6}$$

This equation should be compared with (3.2). While there are some similarities –both are superpositions– one refers to electric fields and the other to "states" of a single photon. Any photon that emerges from the polarizer will necessarily be polarized in the $\hat{\mathbf{x}}$ direction and therefore it will be in the state

$$\text{Beyond the polarizer:} \quad \big|\text{photon}; x\big\rangle \,. \tag{3.7}$$

This can be compared with (3.3) which with the factor $\cos\alpha$ carries information about the amplitude of the wave. Here, for a single photon, there is no room for such a factor.

In the famous Fifth Solvay International Conference of 1927 the world's most notable physicists gathered to discuss the newly formulated quantum theory. Seventeen out of the twenty nine attendees were or became Nobel Prize winners. Einstein, unhappy with the uncertainty in quantum mechanics stated the nowadays famous quote: "God does not play dice", to which Niels Bohr is said to have answered: "Einstein, stop telling God what to do." Bohr was willing to accept the loss of determinism, Einstein was not.

4 Quantum Superpositions

We have already discussed the concept of linearity; the idea that the sum of two solutions representing physical realities represents a new, allowed, physical reality. This superposition of solutions has a straightforward meaning in classical physics. In the case of electromagnetism, for example, if we have two solutions, each with its own electric and magnetic field, the "sum" solution is simply understood: its electric field is the sum of the electric fields of the two solutions and its magnetic field is the sum of the magnetic fields of the two solutions. In quantum mechanics, as we have explained, linearity holds. The interpretation of a superposition, however, is very surprising.

One interesting example is provided by a Mach-Zehnder interferometer; an arrangement of beam splitters, mirrors, and detectors used by Ernst Mach and Ludwig Zehnder in the 1890's to study interference between two beams of light.

A beam splitter, as its name indicates, splits an incident beam into two beams, one that is reflected from the splitter and one that goes through the splitter. Our beam-splitters will be balanced: they split a given beam into two beams of equal intensity (Figure 3). The light that bounces off is called the reflected beam, the light that goes through is called the transmitted beam. The incident beam can hit the beam splitter from the top or from the bottom.

The Mach-Zehnder configuration, shown in Figure 4, has a left beam splitter (BS1) and a right beam splitter (BS2). In between we have the two mirrors, M1 on the top and M2 on the bottom. An incoming beam from the left is split by BS1 into two beams, each of which hits a mirror and is then sent into BS2. At BS2 the beams are recombined and sent into two outgoing beams that go into photon detectors D0 and D1.

It is relatively simple to arrange the beam-splitters so that the incoming beam, upon splitting at BS1 and recombination at BS2 emerges in the top beam which goes into D0. In this arrangement no light at all goes into D1. This requires a precise interference effect at BS2. Note that we have

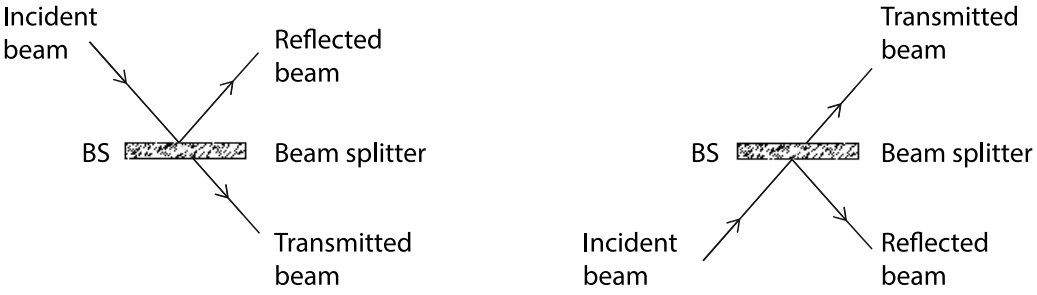

Figure 3: An incident beam hitting a beam-splitter results in a reflected beam and a transmitted beam. Left: incident beam coming from the top. Right: incident beam coming from the bottom.

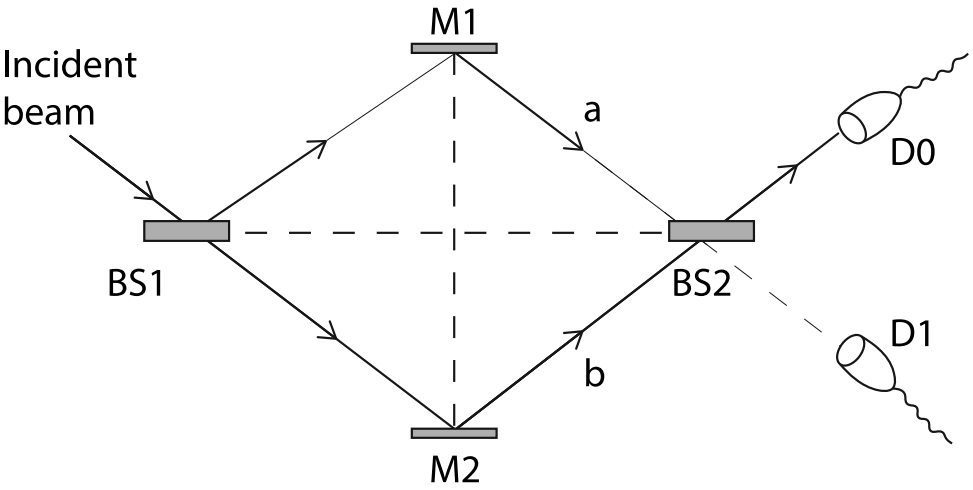

Figure 4: A Mach-Zehnder interferometer consists of two beam splitters BS1 and BS2, two mirrors M1 and M2, and two detectors D0 and D1. An incident beam will be split into two beams by BS1. One beam goes through the upper branch, which contains M1, the other beam goes through the lower branch, which contains M2. The beams on the two branches recombine at BS2 and are then sent into the detectors. The configuration is prepared to produce an interference so that all incident photons end at the detector D0, with none at D1.

two beams incident upon BS2; the top beam is called 'a' and the lower beam is called 'b'. Two contributions go towards D0: the reflection of 'a' at BS2 and the transmission from 'b' at BS2. These two contributions interfere constructively to give a beam going into D0. Two contributions also go towards D1: the transmission from 'a' at BS2 and the reflection from 'b' at BS2. These two can indeed be arranged to interfere destructively to give no beam going into D1.

It is instructive to think of the incoming beam as a sequence of photons that we send into the interferometer, one photon at a time. This shows that, at the level of photons, the interference is not interference of one photon with another photon. Each photon must interfere with *itself* to give the result. Indeed interference between two photons is not possible: destructive interference, for example, would require that two photons end up giving no photon, which is impossible by energy conservation.

Therefore, each photon does the very strange thing of going through both branches of the interferometer! Each photon is in a superposition of two states: a state in which the photon is in the top beam or upper branch, added to a state in which the photon is in the bottom beam or lower branch. Thus the state of the photon in the interferometer is a funny state in which the photon seems to be doing two incompatible things at the same time.

Equation (3.6) is another example of a quantum superposition. The photon state has a component along an x-polarized photon and a component along a y-polarized photon.

When we speak of a wavefunction, we also sometimes call it a state, because the wavefunction specifies the "state" of our quantum system. We also sometimes refer to states as vectors. A quantum state may not be a vector like the familiar vectors in three-dimensional space but it is a vector nonetheless because it makes sense to add states and to multiply states by numbers. Just like vectors can be added, linearity guarantees that adding wavefunctions or states is a sensible thing to do. Just like any vector can be written as a sum of other vectors in many different ways, we will do the same with our states. By writing our physical state as sums of other states we can learn about the properties of our state.

Consider now two states $\big|A\big\rangle$ and $\big|B\big\rangle$. Assume, in addition, that when measuring some property Q in the state $\big|A\big\rangle$ the answer is always a, and when measuring the same property Q in the state $\big|B\big\rangle$ the answer is always b. Suppose now that our physical state $|\Psi\rangle$ is the superposition

$$|\Psi\rangle \;=\; \alpha\big|A\big\rangle + \beta\big|B\big\rangle\,, \qquad \alpha,\beta\in\mathbb{C}\,. \tag{4.1}$$

What happens now if we measure property Q in the system described by the state $|\Psi\rangle$? It may seem reasonable that one gets some intermediate value between a and b, but this is not what happens. A measurement of Q will yield either a or b. There is no certain answer, classical determinism is lost, but the answer is always one of these two values and not an intermediate one. The coefficients α and β in the above superposition affect the probabilities with which we may obtain the two possible values. In fact, the probabilities to obtain a or b

$$\text{Probability}(a)\sim|\alpha|^2\,,\quad \text{Probability}(b)\sim|\beta|^2\,. \tag{4.2}$$

Since the only two possibilities are to measure a or b, the actual probabilities must sum to one and therefore they are given by

$$\text{Probability}(a) \;=\; \frac{|\alpha|^2}{|\alpha|^2+|\beta|^2}\,,\quad \text{Probability}(b) \;=\; \frac{|\beta|^2}{|\alpha|^2+|\beta|^2}\,. \tag{4.3}$$

If we obtain the value a, immediate repeated measurements would still give a, so the state after the measurement must be $|A\rangle$. The same happens for b, so we have

$$\begin{aligned}\text{After measuring } a \;\text{ the state becomes } |\Psi\rangle \;&=|A\rangle\,,\\ \text{After measuring } b \;\text{ the state becomes } |\Psi\rangle \;&=|B\rangle\,.\end{aligned} \tag{4.4}$$

In quantum mechanics one makes the following assumption: *Superposing a state with itself doesn't chance the physics*, nor does it change the state in a non-trivial way. Since superimposing a state with itself simply changes the overall number multiplying it, we have that Ψ and $\alpha\Psi$ represent the same physics for any complex number α different from zero. Thus, letting $\cong$ represent physical equivalence

$$\big|A\big\rangle\cong 2\big|A\big\rangle\cong i\big|A\big\rangle\cong -|A\rangle\,. \tag{4.5}$$

This assumption is necessary to verify that the polarization of a photon state has the expected number of degrees of freedom. The polarization of a plane wave, as one studies in electromagnetism, is described by two real numbers. For this consider an elliptically polarized wave, as shown in Figure 5. At any given point, the electric field vector traces an ellipse whose shape is encoded by the ratio a/b of

the semi-major axes (the first real parameter) and a tilt encoded by the angle θ (the second real parameter). Consider for this a general photon state formed by superposition of the two independent polarization states $|\text{photon}; x\rangle$ and $|\text{photon}; y\rangle$:

$$\alpha|\text{photon}; x\rangle + \beta|\text{photon}; y\rangle\,, \quad \alpha, \beta \in \mathbb{C}\,. \tag{4.6}$$

At first sight it looks as if we have two complex parameters α and β, or equivalently, four real parameters. But since the overall factor does not matter we can multiply this state by $1/\alpha$ to get the equivalent state that encodes all the physics

$$|\text{photon}; x\rangle + \tfrac{\beta}{\alpha}\,|\text{photon}; y\rangle\,, \tag{4.7}$$

showing that we really have one complex parameter, the ratio β/α. This is equivalent to two real parameters, as expected.

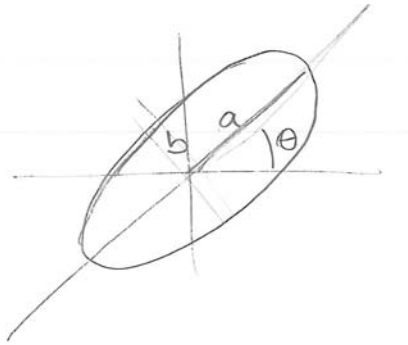

Figure 5: Parameters that define an elliptically polarized state.

Let us do a further example of superposition using electrons. Electrons are particles with spin. Classically, we imagine them as tiny balls spinning around an axis that goes through the particle itself. Once an axis is fixed, the electron has two and only two options: its rotation may be clockwise or counterclockwise about the axis, but in both cases it spins at the same fixed rate. These opposite ways of spinning are called *spin up* and *spin down* along the axis (see Figure 6). The up and down refer to the direction of the angular momentum associated with the rotation, and it is indicated by an arrow. According to quantum mechanics, and as verified by multiple experiments, the same possibilities, up or down, arise *whatever* axis we use to measure the spin of the electron.

Physicists usually set up coordinate systems in space by choosing three orthogonal directions, the directions of the x, y, and z axes. Let us choose to describe our spinning electrons using the z axis. One possible state of an electron is to be spin up along the z axis. Such a state is described as $|\uparrow; z\rangle$, with an arrow pointing up, and the label z indicating that the spin arrow points along the increasing z direction. Another possible state of an electron is spin down along the z axis. Such a state is described as $|\downarrow; z\rangle$, with an arrow pointing down, meaning this time that the spin points along the decreasing z direction. If these two are possible realities, so it would be the state $|\Psi\rangle$ representing the sum

$$|\Psi\rangle \;=\; |\uparrow; z\rangle \,+\, |\downarrow; z\rangle\,.$$

The state $|\Psi\rangle$ is in a superposition of a spin up and a spin down state. What kind of physics does this sum $|\Psi\rangle$ represent? It represents a state in which a measurement of the spin along the z axis would result in two possible outcomes with equal probabilities: an electron with spin up or an electron with spin down. Since we can only speak of probabilities, any experiment must involve repetition until

probabilities can be determined. Suppose we had a large ensemble of such electrons, all of them in the above state $|\Psi\rangle$. As we measured their spin along z, one at a time, we would find about half of them spinning up along z and the other half spinning down along z. There is no way to predict which option will be realized as we measure each electron. It is not easy to imagine superposition, but one may try as follows. An electron in the above state is in a different kind of existence in which it is able to both be spinning up along z and spinning down along z simultaneously! It is in such a ghostly, eerie state, doing incompatible things simultaneously, until its spin is measured. Once measured, the electron must immediately choose one of the two options; we always find electrons either spinning up or spinning down.

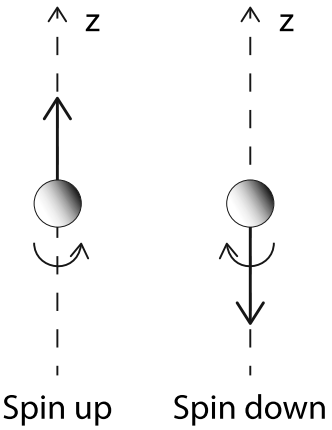

Figure 6: An electron with spin along the z axis. Left: the electron is said to have spin up along z. Right: the electron is said to have spin down along z. The up and down arrows represent the direction of the angular momentum associated with the spinning electron.

A critic of quantum mechanics could suggest a simpler explanation for the above observations. He or she would claim that the following simpler ensemble results in identical experimental results. In the critic's ensemble we have a large number of electrons with 50% of them in the state $|\uparrow; z\rangle$ and 50% of them in the state $|\downarrow; z\rangle$. He or she would then state, correctly, that such an ensemble would yield the same measurements of spins along z as the ensemble of those esoteric $|\Psi\rangle$ states. The new ensemble could provide a simpler explanation of the result without having to invoke quantum superpositions.

Quantum mechanics, however, allows for further experiments that can distinguish between the ensemble of our friendly critic and the ensemble of $|\Psi\rangle$ states. While it would take us too far afield to explain this, if we measured the spin of the electrons in the x direction, instead of z direction, the results would be *different* in the two ensembles. In the ensemble of our critic we would find 50% of the electrons up along x and 50% of the electrons down along x. In our ensemble of $|\Psi\rangle$ states, however, we would find a very simple result: all states pointing up along x. The critic's ensemble is not equivalent to our quantum mechanical ensemble. The critic is thus shown wrong in his or her attempt to show that quantum mechanical superpositions are not required.

5 Entanglement

When we consider superposition of states of *two* particles we can get the remarkable phenomenon called *quantum mechanical entanglement*. Entangled states of two particles are those in which we can't speak separately of the state of each particle. The particles are bound together in a common

state in which they are *entangled* with each other.

Let us consider two non-interacting particles. Particle 1 could be in any of the states

$$\{|u_1\rangle, |u_2\rangle, ...\}\,, \tag{5.1}$$

while particle 2 could be in any of the states

$$\{|v_1\rangle, |v_2\rangle, ...\} \tag{5.2}$$

It may seem reasonable to conclude that the state of the full system, including particle 1 and particle 2 would be specified by stating the state of particle 1 and the state of particle 2. If that would be the case the possible states would be written as

$$|u_i\rangle \otimes |v_j\rangle, \quad i,j \in \mathbb{N}\,, \tag{5.3}$$

for some specific choice of i and j that specify the state of particle one and particle two, respectively. Here we have used the symbol $\otimes$, which means *tensor* product, to combine the two states into a single state for the whole system. We will study $\otimes$ later, but for the time being we can think of it as a kind of product that distributes over addition and obeys simple rules, as follows

$$\begin{aligned}(\alpha_1|u_1\rangle + \alpha_2|u_2\rangle) \otimes (\beta_1|v_1\rangle + \beta_2|v_2\rangle) \;=\; & \alpha_1\beta_1|u_1\rangle \otimes |v_1\rangle + \alpha_1\beta_2|u_1\rangle \otimes |v_2\rangle \\ & + \alpha_2\beta_1|u_2\rangle \otimes |v_1\rangle + \alpha_2\beta_2|u_2\rangle \otimes |v_2\rangle\,.\end{aligned} \tag{5.4}$$

The numbers can be moved across the $\otimes$ but the order of the states must be preserved. The state on the left-hand side –expanded out on the right-hand side– is still of the type where we combine a state of the first particle $(\alpha_1|u_1\rangle + \alpha_2|u_2\rangle)$ with a state of the second particle $(\beta_1|v_1\rangle + \beta_2|v_2\rangle)$. Just like any one of the states listed in (5.3) this state is not entangled.

Using the states in (5.3), however, we can construct more intriguing superpositions. Consider the following one

$$|u_1\rangle \otimes |v_1\rangle + |u_2\rangle \otimes |v_2\rangle\,. \tag{5.5}$$

A state of two particles is said to be **entangled** if it cannot be written in the factorized form $(\cdots)\otimes(\cdots)$ which allows us to describe the state by simply stating the state of each particle. We can easily see that the state (5.5) cannot be factorized. If it could it would have to be with a product as indicated in (5.4). Clearly, involving states like $|u_3\rangle$ or $|v_3\rangle$ that do not appear in (5.5) would not help. To determine the constants $\alpha_1, \alpha_2, \beta_1, \beta_2$ we compare the right hand side of (5.4) with our state and conclude that we need

$$\alpha_1\beta_1 = 1\,, \quad \alpha_1\beta_2 = 0\,, \quad \alpha_2\beta_1 = 0\,, \quad \alpha_2\beta_2 = 1\,. \tag{5.6}$$

It is clear that there is no solution here. The second equation, for example, requires either α_1 or β_2 to be zero. Having $\alpha_1 = 0$ contradicts the first equation, and having $\beta_2 = 0$ contradicts the last equation. This confirms that the state (5.5) is indeed an entangled state. There is no way to describe the state by specifying a state for each of the particles.

Let us illustrate the above discussion using electrons and their spin states. Consider a state of two electrons denoted as $|\uparrow\rangle \otimes |\downarrow\rangle$. As the notation indicates, the first electron, described by the first arrow, is up along z while the second electron, described by the second arrow, is down along z (we omit the label z on the state for brevity). This is not an entangled state. Another possible state is

one where they are doing exactly the opposite: in $|\downarrow\rangle \otimes |\uparrow\rangle$ the first electron is down and the second is up. This second state is also not entangled. It now follows that by superposition we can consider the state

$$|\uparrow\rangle \otimes |\downarrow\rangle \; + \; |\downarrow\rangle \otimes |\uparrow\rangle \, . \tag{5.7}$$

This is a entangled state of the pair of electrons.

Exercise. Show that the above state cannot be factorized and thus is indeed entangled.

In the state (5.7) the first electron is up along z if the second electron is down along z (first term), or the first electron is down along z if the second electron is up along z (second term). There is a correlation between the spins of the two particles; they always point in opposite directions. Imagine that the two entangled electrons are very far away from each other: Alice has one electron of the pair on planet earth and Bob has the other electron on the moon. Nothing we know is connecting these particles but nevertheless the states of the electrons are linked. Measurements we do on the separate particles exhibit correlations. Suppose Alice measures the spin of the electron on earth. If she finds it up along z, it means that the first summand in the above superposition is realized, because in that summand the first particle is up. As discussed before, the state of the two particles immediately becomes that of the first summand. This means that the electron on the moon will *instantaneously* go into the spin down-along-z configuration, something that could be confirmed by Bob, who is sitting in the moon with that particle in his lab. This effect on Bob's electron happens before a message, carried with the speed of light, could reach the moon telling him that a measurement has been done by Alice on the earth particle and the result was spin up. Of course, experiments must be done with an ensemble that contains many pairs of particles, each pair in the same entangled state above. Half of the times the electron on earth will be found up, with the electron on the moon down and the other half of the times the electron on earth will be found down, with the electron on the moon up.

Our friendly critic could now say, correctly, that such correlations between the measurements of spins along z could have been produced by preparing a *conventional* ensemble in which 50% of the pairs are in the state $|\uparrow\rangle \otimes |\downarrow\rangle$ and the other 50% of the pairs are in the state $|\downarrow\rangle \otimes |\uparrow\rangle$. Such objections were dealt with conclusively in 1964 by John Bell, who showed that if Alice and Bob are able to measure spin in *three* arbitrary directions, the correlations predicted by the quantum entangled state are different from the classical correlations of *any* conceivable conventional ensemble. Quantum correlations in entangled states are very subtle and it takes sophisticated experiments to show they are not reproducible as classical correlations. Indeed, experiments with entangled states have confirmed the existence of quantum correlations. The kind of instantaneous action at a distance associated with measurements on well-separated entangled particles does not lead to paradoxes nor, as it may seem, to contradictions with the ideas of special relativity. You cannot use quantum mechanical entangled states to send information faster than the speed of light.

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

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Chapter 2: Experiments with photons

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1 Mach-Zehder Interferometer

We have discussed before the Mach-Zehnder interferometer, which we show again in Figure 1. It contains two beam-splitters BS1 and BS2 and two mirrors. Inside the interferometer we have two beams, one going over the upper branch and one going over the lower branch. This extends beyond BS2: the upper branch continues to D0 while the lower branch continues to D1.

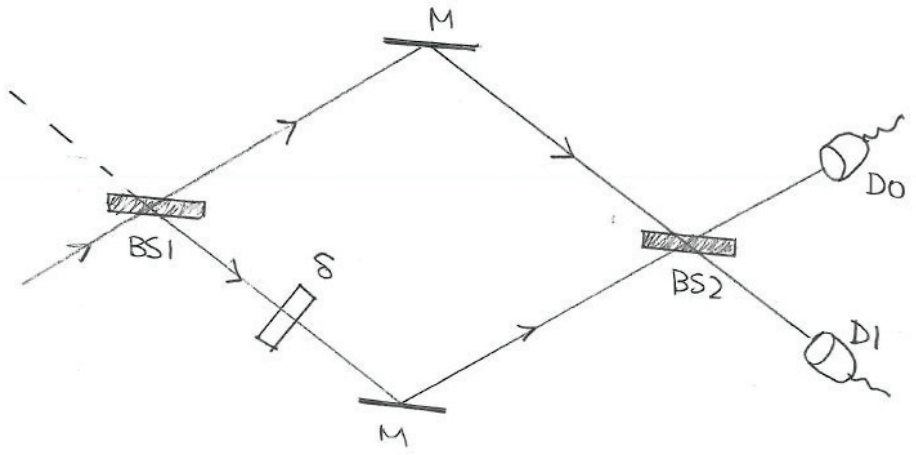

Figure 1: The Mach-Zehnder Interferometer

Vertical cuts in the above figure intersect the two beams and we can ask what is the probability to find a photon in each of the two beams at that cut. For this we need two probability *amplitudes*, or two complex numbers, whose norm-squared would give probabilities. We can encode this information in a two component vector as

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} . \tag{1.1}$$

Here α is the probability amplitude to be in the upper beam and β the probability amplitude to be in the lower beam. Therefore, $|\alpha|^2$ would be the probability to find the photon in the upper beam and $|\beta|^2$ the probability to find the photon in the lower beam. Since the photon must be found in either one of the beams we must have

$$\big|\alpha\big|^2 + \big|\beta\big|^2 = 1\,. \tag{1.2}$$

Following this notation, we would have for the cases when the photon is definitely in one or the other beam:

$$\text{photon on upper beam: } \begin{pmatrix}1\\0\end{pmatrix}, \qquad \text{photon on bottom beam : } \begin{pmatrix}0\\1\end{pmatrix}. \tag{1.3}$$

We can view the state (1.1) as a superposition of these two simpler states using the rules of vector addition and multiplication:

$$\begin{pmatrix}\alpha\\\beta\end{pmatrix} = \begin{pmatrix}\alpha\\0\end{pmatrix} + \begin{pmatrix}0\\\beta\end{pmatrix} \;=\; \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix}. \tag{1.4}$$

In the interferometer shown in Figure 1 we included in the lower branch a 'phase shifter', a piece of

Figure 2: A phase shifter of phase factor $e^{i\delta}$. The amplitude gets multiplied by the phase.

material whose only effect is to multiply the probability amplitude by a fixed phase $e^{i\delta}$ with $\delta \in \mathbb{R}$. As shown in Figure 2, the probability amplitude α to the left of the device becomes $e^{i\delta}\alpha$ to the right of the device. Since the norm of a phase is one, the phase-shifter does not change the probability to find the photon. When the phase δ is equal to π the effect of the phase shifter is to change the sign of the wavefunction since $e^{i\pi} = -1$.

Let us now consider the effect of beam splitters in detail. If the incoming photon hits a beam-splitter from the top, we consider this photon to belong to the upper branch and represent it by $\begin{pmatrix}1\\0\end{pmatrix}$. If the incoming photon hits the beam-splitter from the bottom, we consider this photon to belong to the lower branch, and represent it by $\begin{pmatrix}0\\1\end{pmatrix}$. We show the two cases in Figure 3. The effect of the beam splitter is to give an output wavefunction for each of the two cases:

$$\text{Left BS: } \begin{pmatrix}1\\0\end{pmatrix} \to \begin{pmatrix}s\\t\end{pmatrix}, \qquad \text{Right BS: } \begin{pmatrix}0\\1\end{pmatrix} \to \begin{pmatrix}u\\v\end{pmatrix}. \tag{1.5}$$

As you can see from the diagram, for the photon hitting from above, s may be thought as a reflection amplitude and t as a transmission coefficient. Similarly, for the photon hitting from below, v may be thought as a reflection amplitude and u as a transmission coefficient. The four numbers s, t, u, v, by linearity, characterize completely the beam splitter. They can be used to predict the output given any incident photon, which may have amplitudes to hit both from above and from below. Indeed, an incident photon state $\begin{pmatrix}\alpha\\\beta\end{pmatrix}$ would give

$$\begin{pmatrix}\alpha\\\beta\end{pmatrix} = \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix} \quad\to\quad \alpha\begin{pmatrix}s\\t\end{pmatrix} + \beta\begin{pmatrix}u\\v\end{pmatrix} \;=\; \begin{pmatrix}\alpha s + \beta u\\ \alpha t + \beta v\end{pmatrix} \;=\; \begin{pmatrix}s & u\\ t & v\end{pmatrix}\begin{pmatrix}\alpha\\\beta\end{pmatrix}. \tag{1.6}$$

In summary, we see that the BS produces the following effect

$$\begin{pmatrix}\alpha\\\beta\end{pmatrix} \quad\to\quad \begin{pmatrix}s & u\\ t & v\end{pmatrix}\begin{pmatrix}\alpha\\\beta\end{pmatrix}. \tag{1.7}$$

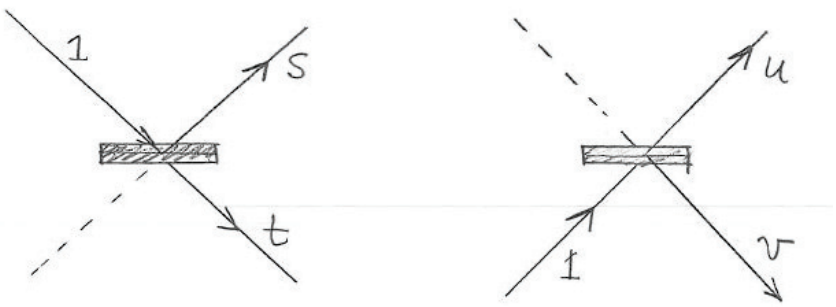

Figure 3: Left: A photon incident from the top; s and t are the reflected and transmitted amplitudes, respectively. Right: A photon incident from the bottom; v and u are the reflected and transmitted amplitudes, respectively.

We can represent the action of the beam splitter as matrix multiplication on the incoming wavefunction, with the two-by-two matrix

$$\begin{pmatrix} s & u \\ t & v \end{pmatrix} . \tag{1.8}$$

We must now figure out the constraints on s, t, u, v. Because probabilities must add up to one, equation (1.5) implies that

$$\begin{aligned} |s|^2 + |t|^2 &= 1 , & (1.9) \\ |u|^2 + |v|^2 &= 1 . & (1.10) \end{aligned}$$

The kind of beam splitters we use are called balanced, which means that reflection and transmission probabilities are the same. So all four constants must have equal norm-squared:

$$|s|^2 = |t|^2 = |u|^2 = |v|^2 = \tfrac{1}{2} . \tag{1.11}$$

Let's try a guess for the values. Could we have

$$\begin{pmatrix} s & u \\ t & v \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} ? \tag{1.12}$$

This fails if acting on normalized wavefunctions (or column vectors) does not yield normalized wavefunctions. So we try with a couple of wavefunctions

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} , \qquad \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} . \tag{1.13}$$

While the first example works out, the second does not, as $|1|^2 + |1|^2 = 2 \neq 1$. An easy fix is achieved by changing the sign of v:

$$\begin{pmatrix} s & u \\ t & v \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} . \tag{1.14}$$

Let's check that this matrix works in general. Thus acting on a state $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ with $|\alpha|^2+|\beta|^2=1$ we find

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}\alpha+\beta\\ \alpha-\beta\end{pmatrix}. \tag{1.15}$$

Indeed the resulting state is well normalized. The total probability is what we expect

$$\begin{aligned}\tfrac{1}{2}\big|\alpha+\beta\big|^2+\tfrac{1}{2}\big|\alpha-\beta\big|^2 &=\tfrac{1}{2}(\big|\alpha\big|^2+\big|\beta\big|^2+\alpha\beta^*+\alpha^*\beta)+\tfrac{1}{2}(\big|\alpha\big|^2+\big|\beta\big|^2-\alpha\beta^*-\alpha^*\beta)\\ &=\big|\alpha\big|^2+\big|\beta\big|^2\;=\;1\,.\end{aligned} \tag{1.16}$$

The minus sign in the bottom right entry of (1.14) means that a photon incident from below, as it is reflected, will have its amplitude changed by a sign or equivalently a phase shift by π (check this!). This effect, of course, is realized in practice. A typical beam splitter consists of a glass plate with a reflective dielectric coating on one side. The refractive index of the coating is chosen to be intermediate between that of glass and that of air. A reflection causes a phase shift only when light encounters a material of higher refractive index. This is the case in the transition of air to coating, but not in the transition from glass to coating. Thus the beam splitter represented by (1.14) would have its coating on the bottom side. Transmitted waves have no phase shift.

Another possibility for a beam splitter matrix is

$$\frac{1}{\sqrt{2}}\begin{pmatrix}-1 & 1\\ 1 & 1\end{pmatrix}, \tag{1.17}$$

which would be realized by a dielectric coating on the top side. You can quickly check that, like the previous matrix, its action also conserves probability. We will call the left beam-splitter BS1 and the right beam splitter BS2 and their respective matrices will be

$$\text{BS1}:\;\;\frac{1}{\sqrt{2}}\begin{pmatrix}-1 & 1\\ 1 & 1\end{pmatrix},\quad \text{BS2}:\;\;\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}. \tag{1.18}$$

The two beam splitters are combined to form the interferometer shown in Figure 4. If we now assume an input photon wavefunction $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ from the left, the output wavefunction that goes into the detectors is obtained by acting first with the BS1 matrix and then with the BS2 matrix:

$$\text{input}:\;\begin{pmatrix}\alpha\\ \beta\end{pmatrix}\quad\text{output:}\;\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}-1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}=\tfrac{1}{2}\begin{pmatrix}0 & 2\\ -2 & 0\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}=\begin{pmatrix}\beta\\ -\alpha\end{pmatrix}. \tag{1.19}$$

With the help of this result, for any input photon state we can write immediately the output photon state that goes into the detectors.

If the input photon beam is $\begin{pmatrix}0\\ 1\end{pmatrix}$, the output from the interferometer is $\begin{pmatrix}1\\ 0\end{pmatrix}$, and therefore a photon will be detected at D0. This is shown in Figure 5. We can make a very simple table with the possible outcomes and their respective probabilities P:

Outcome	P
photon at DO	1
photon at D1	0

(1.20)

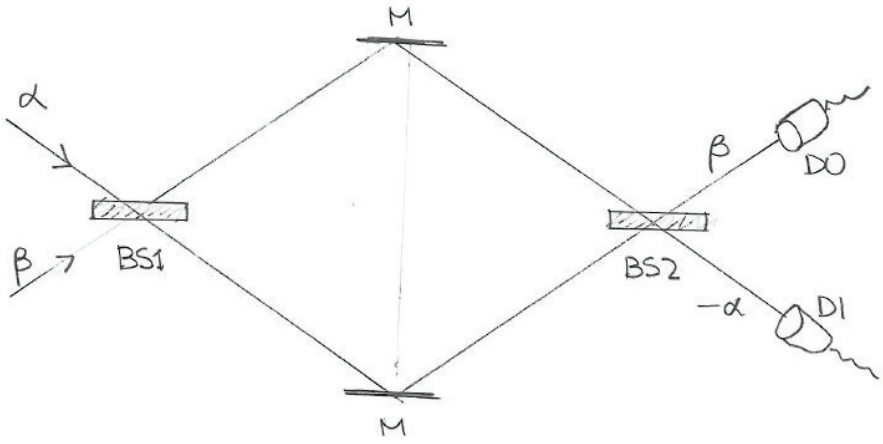

Figure 4: The Mach-Zehnder interferometer with input and output wavefunctions indicated.

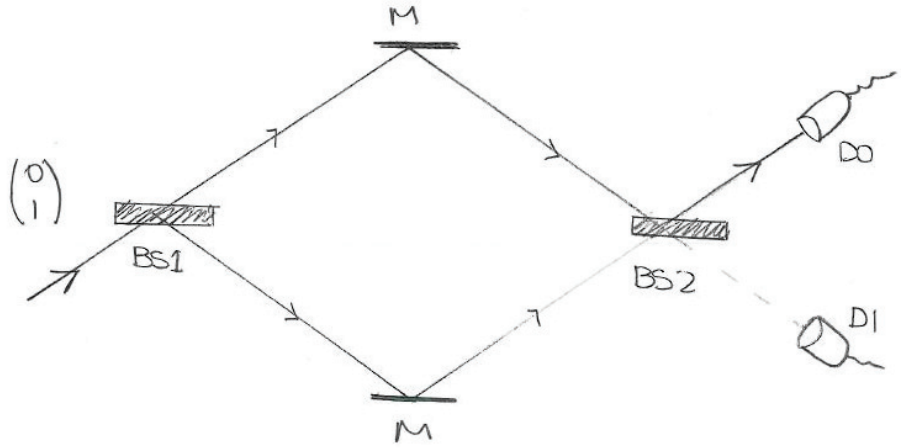

Figure 5: Incident photon from below will go into D0.

Now, block the lower path, as indicated in Figure 6. What happens then? It is best to track down things systematically. The input beam, acted by BS1 gives

$$\frac{1}{\sqrt{2}}\begin{pmatrix}-1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \tfrac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}. \tag{1.21}$$

This is indicated in the figure, to the right of BS1. Then the lower branch is stopped, while the upper branch continues. The upper branch reaches BS2, and here the input is $\begin{pmatrix}\frac{1}{\sqrt{2}}\\0\end{pmatrix}$, because nothing is coming from the lower branch. We therefore get an output

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\0\end{pmatrix} = \begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\end{pmatrix}. \tag{1.22}$$

In this experiment there are three possible outcomes: the photon can be absorbed by the block, or

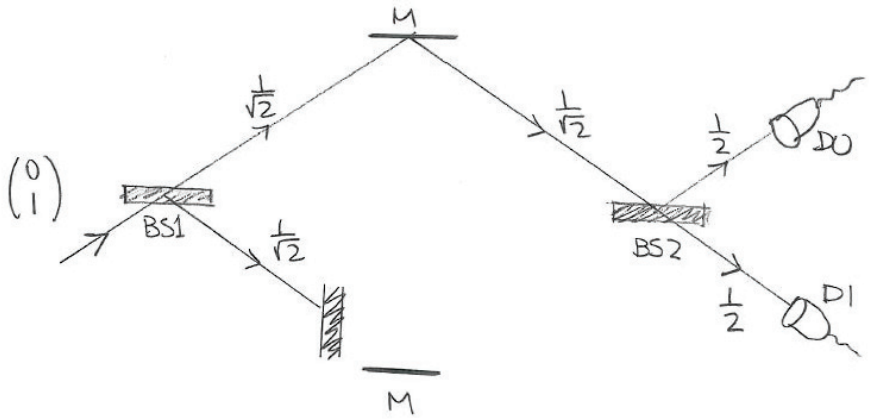

Figure 6: The probability to detect the photon at D1 can be changed by blocking one of the paths.

can go into any of the two detectors. As we see in the diagram, the probabilities are:

Outcome	P
photon at block	$\frac{1}{2}$
photon at D0	$\frac{1}{4}$
photon at D1	$\frac{1}{4}$

(1.23)

It is noteworthy that before blocking the lower path we could not get a photon to D1. The probability to reach D1 is now 1/4 and was increased by blocking a path.

2 Elitzur-Vaidman Bombs

To see that allowing the photon to reach D1 by blocking a path is very strange, we consider an imaginary situation proposed by physicists Avshalom Elitzur and Lev Vaidman, from Tel-Aviv University, in Israel. They imagined bombs with a special type of trigger: a photon detector. A narrow tube goes across each bomb and in the middle of the tube there is a photon detector. To detonate the bomb one sends a photon into the tube. The photon is then detected by the photon detector and the bomb explodes. If the photon detector is defective, however, the photon is not detected at all. It propagates freely through the tube and comes out of the bomb. The bomb does not explode.

Here is the situation we want to address. Suppose we have a number of Elitzur-Vaidman (EV) bombs, but we know that some of them have become defective. How could we tell if a bomb is operational without detonating it? Assume, for the sake of the problem, that we are unable to examine the detector without destroying the bomb.

We seem to be facing an impossible situation. If we send a photon into the detector tube and nothing happens we know the bomb is defective, but if the bomb is operational it would simply explode. It seems impossible to confirm that the photon detector in the bomb is working without testing it. Indeed, it is impossible in classical physics. It is not impossible in quantum mechanics, however. As we will see, we can perform what can be called an interaction-free measurement!

We now place an EV bomb on the lower path of the interferometer, with the detector tube properly aligned. Suppose we send in a photon as pictured. If the bomb is defective it is as if there is no detector, the lower branch of the interferometer is free and all the photons that we send in will end up in D0,

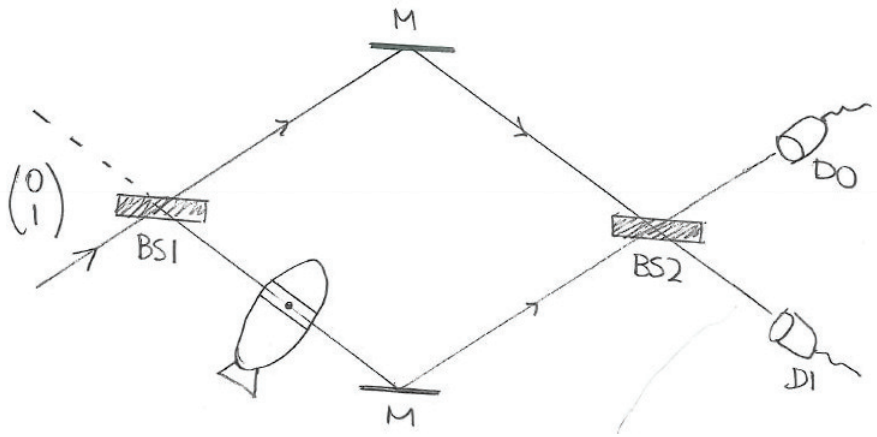

Figure 7: A Mach-Zehnder interferometer and an Elitzur-Vaidman bomb inserted on the lower branch, with the detector tube properly aligned. If the bomb is faulty all incident photons will end up at D0. If a photon ends up at D1 we know that the bomb is operational, even though the photon never went into the bomb detector!

just as they did in Figure 5.

Outcome	P
photon at D0 no explosion	1
photon at D1 no explosion	0
bomb explodes	0

(2.24)

If the bomb is working, on the other hand, we have the situation we had in Figure 6, where we placed a block in the lower branch of the interferometer:

Outcome	P
bomb explodes	$\frac{1}{2}$
photon at D0 no explosion	$\frac{1}{4}$
photon at D1 no explosion	$\frac{1}{4}$

(2.25)

Assume the bomb is working. Then 50% of the times the photon will hit it and it will explode, 25% of the time the photon will end in D0 and we can't tell if it is defective or not. But 25% of the time the photon will end in D1, and since this was impossible for a faulty bomb, we have learned that the bomb is operational! We have learned that even though the photon never made it through the bomb; it ended on D1. If you think about this you will surely realize it is extremely surprising and counterintuitive. But it is true, and experiments (without using bombs!) have confirmed that this kind of interaction-free measurement is indeed possible.

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

PARTICLE NATURE OF LIGHT AND WAVE NATURE OF MATTER

B. Zwiebach
February 16, 2016

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1 Photoelectric Effect

The photoelectric effect was first observed by Heinrich Hertz in 1887. When polished metal plates are irradiated, he observed, they may emit electrons, then called "photo-electrons". The emitted electrons thus produce a *photoelectric current*. The key observations were:

- There is a threshold frequency ν_0. Only for frequencies $\nu > \nu_0$ is there a photoelectric current. The frequency ν_0 depends on the metal and the configuration of the atoms at the surface. It is also affected by inhomogeneities.
- The magnitude of the photoelectric current is proportional to the intensity of the light source.
- Energy of the photoelectrons is *independent* of the intensity of the light source.

A natural explanation for the features in this effect didn't come until 1905, when Einstein explained the above features by postulating that the energy in light is carried by discrete quanta (later called photons) with energy $h\nu$. Here h is Planck's constant, the constant used by Planck to to produce a fit for the blackbody energy as a function of frequency.

Figure 1: Electrons in a metal are bound. If the photon energy is greater than the work function W an electron may be ejected.

A given material has a characteristic energy W, called the *work function*, which is the minimum energy required to eject an electron. This is not easily calculated because it is the result of an

interaction of many electrons with the background of atoms. It is easily measured, however. When the surface of the material is irradiated, electrons in the material absorb the energy of the incoming photons. If the energy imparted on an electron by the absorption of a single photon is greater than the work function W, then the electron is ejected with kinetic energy E_{e^-} equal to the difference of the photon energy and the work function:

$$E_{e^-} \;=\; \tfrac{1}{2}mv^2 \;=\; h\nu - W \;=\; E_\gamma - W. \tag{1.1}$$

This equation, written by Einstein explains the experimental features noted above, once we assume that the quanta act on individual electrons to eject them. The threshold frequency is defined by

$$h\nu_0 = W\,, \tag{1.2}$$

as it leads to a photoelectron with zero energy. For $\nu > \nu_0$ the electrons will be ejected. Increasing the intensity of the light source increases the rate that photons arrive, which will increase the magnitude of the current, but will not change the energy of the photoelectrons because it does not change the energy of each incoming quanta.

Equation (1.2) allowed Einstein to make a prediction: The kinetic energy of the photo-electrons increases linearly with the frequency of light. Einstein's prediction was confirmed experimentally by Millikan (1915) who measured carefully the photoelectron energies and confirmed their linear dependence on the energy. Millikan's careful work allowed him to determine the value of Planck's constant $\hbar$ to better than 1% accuracy! Still, skepticism remained and physicists were not yet convinced about the particle nature of these light quanta.

Example: Consider UV light with wavelength $\lambda = 290$nm incident on a metal with work function $W = 4.05$eV What is the energy of the photo-electron and what is its speed?

Solution: It is useful to solve these problems without having to look up constants. For this try recalling this useful relation

$$\hbar c \;=\; 197.33\ \text{MeV.fm}\,, \qquad \hbar \equiv \frac{h}{2\pi}\,, \tag{1.3}$$

where MeV $= 10^6$eV and fm$= 10^{-15}$m. Let us use this to compute the photon energy. In this case,

$$E_\gamma = h\nu = \; 2\pi\hbar\frac{c}{\lambda} \;=\; \frac{2\pi\cdot 197.33\ \text{MeV.fm}}{290\times 10^{-9}\text{m.}} \;=\; \frac{2\pi\cdot 197.33}{290}\ \text{eV} \;\approx\; 4.28\,\text{eV}, \tag{1.4}$$

and thus

$$E_{e^-} = E_\gamma - W = 0.23\,\text{eV}. \tag{1.5}$$

To compute the energy we set

$$0.23\,\text{eV} \;=\; \tfrac{1}{2}m_e v^2 \;=\; \tfrac{1}{2}(m_e c^2)\left(\tfrac{v}{c}\right)^2 \tag{1.6}$$

Recalling that $m_e c^2 \simeq 511,000$eV one finds

$$\tfrac{0.46}{511000} \;=\; \left(\tfrac{v}{c}\right)^2 \quad\rightarrow\quad \tfrac{v}{c} \;=\; 0.0009488\,. \tag{1.7}$$

With and $c = 300,000$ Km/s we finally get $v \simeq 284.4\,$Km/s.

This is a good point to consider units, in particular the units of h. We can ask: Is there a physical quantity that has the units of h. The answer is yes, as we will see now. From the equation $E = h\nu$, we have

$$[h] = \left[\frac{E}{\nu}\right] = \frac{ML^2/T^2}{1/T} = L\cdot M\frac{L}{T}\,, \tag{1.8}$$

where $[\cdot]$ gives the units of a quantity, and M, L, T are units of mass, length, and time, respectively. We have written the right-most expression as a product of units of length and momentum. Therefore

$$[h] \;=\; [\mathbf{r} \times \mathbf{p}] = [\mathbf{L}]. \tag{1.9}$$

We see that h has units of angular momentum! Indeed for a spin one-half particle, the magnitude of the spin angular momentum is $\frac{1}{2}\hbar$.

With $[h] = [r][p]$ we also see that one has a canonical way to associate a length to any particle of a given mass m. Indeed, using the speed of light, we can construct the momentum $p = mc$, and then the length ℓ is obtained from the ratio h/p. This actually is the **Compton wavelength** ℓ_C of a particle:

$$\lambda_C = \frac{h}{mc} \tag{1.10}$$

then has units of length; this is called the *Compton wavelength* of a particle of mass m. Note that this length is independent of the velocity of the particle. The de Broglie wavelength of the particle uses the true momentum of the particle, not mc! Thus, Compton and de Broglie wavelengths should not be confused!

It is possible to get some physical intuition for the Compton wavelength λ_C of a particle. We claim that λ_C *is the wavelength of a photon whose energy is equal to the rest energy of the particle.* Indeed we would have

$$mc^2 \;=\; h\nu \;=\; h\,\tfrac{c}{\lambda} \quad \rightarrow \quad \lambda = \frac{h}{mc}\,, \tag{1.11}$$

confirming the claim. Suppose you are trying to localize a point particle of mass m. If you use light, the possible accuracy in the position of the particle is roughly the wavelength of the light. Once we use light with $\lambda < \lambda_C$ the photons carry more energy than the rest energy of the particle. It is possible then that the energy of the photons go into creating more particles of mass m, making it difficult, if not impossible to localize the particle. The Compton wavelength is the length scale at which we need *relativistic quantum field theory* to take into account the possible processes of particle creation and annihilation.

Let us calculate the Compton wavelength of the electron:

$$\lambda_C(e) = \frac{h}{m_e c} \;=\; \frac{2\pi\hbar c}{m_e c^2} \;=\; \frac{2\pi \cdot 197.33\,\text{MeV.fm}}{0.511\,\text{MeV}} \;=\; 2426\,\text{fm} \;=\; 2.426\,\text{pm}. \tag{1.12}$$

This length is about 20 times smaller than the Bohr radius (53 pm.) and about two-thousand times the size of a proton (1 fm.). The Compton wavelength of the electron appears in the formula for the change of photon wavelength in the process called Compton scattering.

2 Compton Scattering

Originally Einstein did not make clear that the light quantum meant a particle of light. In 1916, however, he posited that the quantum would carry momentum as well as energy, making the case for a particle much clearer. In relativity, the energy, momentum, and rest mass of a particle are related by

$$E^2 - p^2c^2 \;=\; m^2c^4. \tag{2.13}$$

(Compare this with the classical equation $E = p^2/2m$.) Of course, one can also express the energy and momentum of the particle in terms of the velocity:

$$E = \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}}, \quad \mathbf{p} = \frac{m\mathbf{v}}{\sqrt{1-\frac{v^2}{c^2}}}. \tag{2.14}$$

You should use these expressions to confirm that (2.13) holds ($|\mathbf{p}| = p$). A particle that moves with the speed of light, like the photon, must have zero rest mass, otherwise its energy and momentum would be infinite due to the vanishing denominators. With the rest mass set to zero, equation (2.13) gives the relation between the photon energy E_γ and the photon momentum p_γ:

$$E_\gamma = p_\gamma c. \tag{2.15}$$

Then, using $\lambda\nu = c$, we reach

$$p_\gamma = \frac{E_\gamma}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}. \tag{2.16}$$

We will see this relation again later when we discuss matter waves.

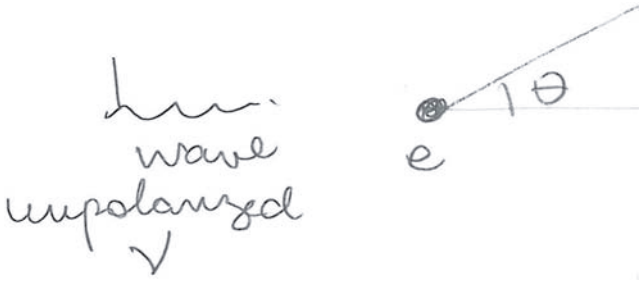

Figure 2: Unpolarized light incident on an electron scatters into an angle θ. Classically, this is described by Thomson scattering. The light does not change frequency during this process.

Compton carried out experiments (1923–1924) scattering X-rays off a carbon target. X-rays correspond to photon energies in the range from 100 eV to 100 KeV. The goal was scattering X-ray photons off free electrons, and with some qualification, the electrons in the atoms behave this way.

The classical counterpart of the Compton experiment is the scattering of electromagnetic waves off free electrons, called *Thompson scattering*. Here an electromagnetic wave is incident on a electron. The electric field of the wave shakes the electron which oscillates with the frequency of the incoming field. The electron oscillation produces a radiated field, of the same frequency as that of the incoming radiation. In classical Thomson scattering the differential scattering cross section is given by

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{mc^2}\right)^2 \tfrac{1}{2}\left(1+\cos^2\theta\right), \tag{2.17}$$

where θ is the angle between the incident and scattered wave, with the radiated energy at the same frequency as the incoming light. This is shown in Figure 2. The cross-section has units of length-squared, or area, as it should. It represents the area that would extract from the incoming plane wave the amount of energy that is scattered by the electron. Indeed the quantity $e^2/(mc^2)$ is called the classical electron radius and it is about 2.8 fm! not much bigger than a proton!

If we treat the light as photons, the elementary process going on is a collision between two particles; an incoming photon and a roughly stationary electron. Two facts can be quickly demonstrated:

- The photon cannot be absorbed by the electron. It is inconsistent with energy and momentum conservation (exercise)
- The photon must lose some energy and thus the final photon wavelength λ_f must be larger than the initial photon wavelength λ_i. This is clear in the laboratory frame, where the initially stationary electron must recoil and thus acquire some kinetic energy.

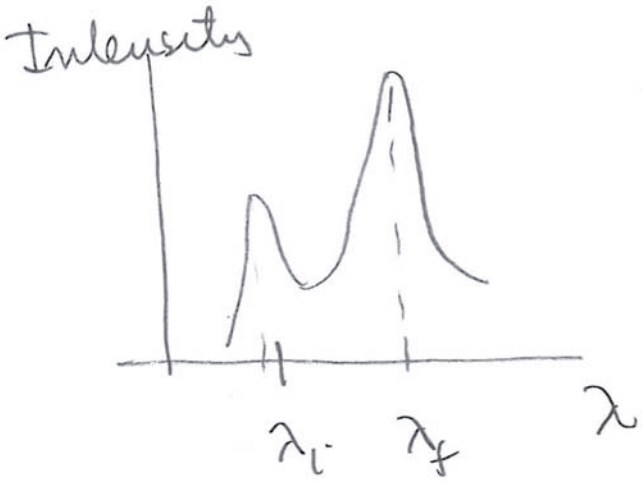

Figure 3: The results of Compton's scattering experiment. The incident photon wavelength is λ_i, and the scattered photon wavelength is $\lambda_f \simeq \lambda_i + \ell_C$, corresponding to $\theta = 90°$.

Indeed, Compton's observations did not agree with the predictions of Thompson scattering: the X-rays changed frequency after scattering. A calculation using energy and momentum conservation shows that the change of wavelength is correlated with the angle between the scattered photon and the original photon:

$$\lambda_f = \lambda_i + \frac{h}{m_e c}(1 - \cos\theta) \;=\; \lambda_i + \ell_C\,(1 - \cos\theta)\,. \tag{2.18}$$

Note that appearance of the Compton wavelength of the electron, the particle the photon scatters off from. The maximum energy loss for the photon occurs at $\theta = \pi$, where

$$\lambda_f(\theta = 180°) = \lambda_i + 2\lambda_C\,. \tag{2.19}$$

The maximum possible change in wavelength is $2\lambda_C$. For $\theta = \frac{\pi}{2}$ the change of wavelength is exactly ℓ_C

$$\lambda_f(\theta = 90°) = \lambda_i + \lambda_C\,. \tag{2.20}$$

Compton's experiment used molybdenum X-rays with energy and wavelength

$$E_\gamma \approx 17.5\,\text{keV}\,, \qquad \lambda_i = 0.0709\,\text{nm}\,, \tag{2.21}$$

incident on a carbon target. Placing the detector at an angle $\theta = 90°$ the plot of the intensity (or number of photons scattered) as a function of wavelength is shown in Figure 2. One finds a peak for for $\lambda_f = 0.0731$ nm, but also a second peak at the original wavelength $\lambda_i = 0.0709$ nm.

The peak at λ_f is the expected one: $\lambda_f - \lambda_i \simeq 2.2\,\text{pm}$, which is about the Compton wavelength of 2.4 pm. Given that the photons have energies of 17 KeV and the bound state energies of carbon

are about 300 eV, the expected peak represents instances where the atom is ionized by the collision and it is a fine approximation to consider the ejected electrons. The peak at λ_i represents a process in which an electron receives some momentum from the photon but still remains bound. This is not very unlikely: the typical momentum of a bound electron is actually comparable to the momentum of the photon. In this case the photon scatters at 90° and the recoil momentum is carried by the whole atom. The relevant Compton wavelength is therefore that of the atom. Since the mass of the carbon atom is several thousands of times larger than the mass of the electron, the Compton wavelength of the atom is much smaller than the electron Compton wavelength and there should be no detectable change in the wavelength of the photon.[1]

3 Matter Waves

As we have seen, light behaves as both a particle and a wave. This kind of behavior is usually said to be a **duality:** the complete reality of the object is captured using *both* the wave and particle features of the object. The photon is a particle of energy E_γ, but has frequency ν which is a wave attribute, with $E = h\nu$. It is a particle with momentum p_γ but it also has a wavelength λ, a wave attribute, given by (2.16)

$$\lambda = \frac{h}{p_\gamma}. \tag{3.22}$$

In 1924, Louis de Broglie proposed that the wave/particle duality of the photon was universal, and thus valid for matter particles too. In this way he conjectured the *wave nature of matter*. Inspired by (3.22) de Broglie postulated that associated to a matter particle with momentum p there is a plane wave of wavelength λ given by

$$\lambda = \frac{h}{p}. \tag{3.23}$$

This is a fully quantum property: if $h \to 0$, then $\lambda \to 0$, and the particles have no wave properties. And exciting consequence of this is that matter particles can diffract or interfere! In the famous Davisson-Germer experiment (1927) electrons are strike a metal surface and one finds that at certain angles there are peaks in the intensity of the scattered electrons. The peaks showed the effect of constructive interference from scattering off the lattice of atoms in the metal, demonstrating the wave nature of the electrons. One can also do two-slit interference with electrons, and the experiment can be done shooting one electron at a time. A recent experiment [arXiv:1310.8343] by Eibenberger *et.al* reports interference using molecules with 810 atoms and mass exceeding 10 000 amu (that's 20 million times the mass of the electron!)

The de Broglie wavelength can be calculated to estimate if quantum effects are important. Consider for this purpose a particle of mass m and momentum p incident upon an object of size x, as illustrated in Figure 3. Let $\lambda = h/p$ denote the de Broglie wavelength of the particle. The wave nature of the particle is not important if λ is much smaller than x. Thus, the "classical approximation," in which wave effects are negligible, requires

$$\text{Wave effects negligible:} \qquad \frac{\lambda}{x} \ll 1. \tag{3.24}$$

Using $\lambda = h/p$, this yields

$$\text{Wave effects negligible:} \qquad x\,p \gg h\,, \tag{3.25}$$

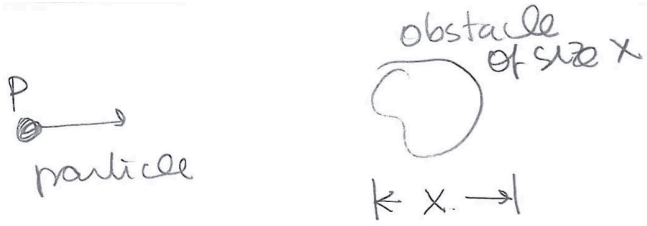

Figure 4: A particle of momentum p incident on an obstacle of size x.

a relation in which both sides have units of angular momentum.

Classical behavior is a subtle limit of quantum mechanics: a classical electromagnetic field requires a large number of photons. Any state with an exact, fixed number of photons, even if large, is not classical, however. Classical electromagnetic states are so-called coherent states, in which the number of photons fluctuates.

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

[1]Thanks to V. Vuletic for a clarification of this point.

Lecture 4

B. Zwiebach
February 18, 2016

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2 Phase and Group Velocities **4**

3 Choosing the wavefunction for a free particle **6**

1 de Broglie wavelength and Galilean transformations

We have seen that to any free particle with momentum $\mathbf{p}$, we can associate a plane wave, or a "matter wave", with de Broglie wavelength $\lambda = h/p$, with $p = |\mathbf{p}|$. The question is, *waves of what*? Well, this wave is eventually recognized as an example of what one calls the *wavefunction*. The wavefunction, as we will see is governed by the Schrödinger equation. As we have hinted, the wavefunction gives us information about probabilities, and we will develop this idea in detail.

Does the wave have directional or polarization properties like electric and magnetic fields in an electromagnetic wave? Yes, there is an analog of this, although we will not delve into it now. The analog of polarization corresponds to spin! The effects of spin are negligible in many cases (small velocities, no magnetic fields, for example) and for this reason, we just use a scalar wave, a complex number

$$\Psi(\mathbf{x}, t) \in \mathbb{C} \tag{1.1}$$

that depends on space and time. A couple of obvious questions come to mind. Is the wavefunction measurable? What kind of object is it? What does it describe? In trying to get intuition about this, let's consider how different observers perceive the de Broglie wavelength of a particle, which should help us understand what kind of waves we are talking about. Recall that

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k, \tag{1.2}$$

where k is the wavenumber. How would this wave behave under a change of frame?

We therefore consider two frames S and S' with the x and x' axes aligned and with S' moving to the right along the $+x$ direction of S with constant velocity v. At time equal zero, the origins of the two reference frames coincide.

The time and spatial coordinates of the two frames are related by a *Galilean transformation*, which states that

$$x' = x - vt, \quad t' = t\,. \tag{1.3}$$

Indeed time runs at the same speed in all Galilean frames and the relation between x and x' is manifest from the arrangement shown in Fig. 1.

Now assume both observers focus on a particle of mass m moving with nonrelativistic speed. Call the speed and momentum in the S frame $\widetilde{v}$ and $p = m\widetilde{v}$, respectively. It follows by differentiation with

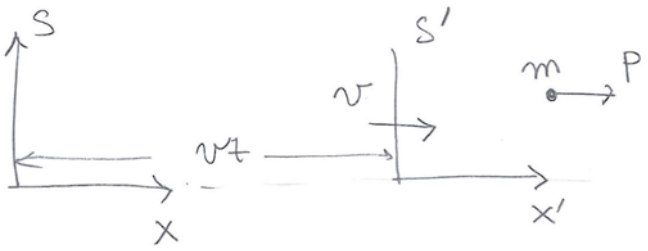

Figure 1: The S' frame moves at speed v along the x-direction of the S frame. A particle of mass m moves with speed $\widetilde{v}$, and thus momentum $p = m\widetilde{v}$, in the S frame.

respect to $t = t'$ of the first equation in (1.3) that

$$\frac{dx'}{dt'} \;=\; \frac{dx}{dt} - v\,, \tag{1.4}$$

which means that the particle velocity $\widetilde{v}'$ in the S' frame is given by

$$\widetilde{v}' \;= \widetilde{v} - v\,. \tag{1.5}$$

Multiplying by the mass m we find the relation between the momenta in the two frames

$$p' \;=\; p - mv. \tag{1.6}$$

The momentum p' in the S' frame can be appreciably different from the momentum p in the S frame. Thus the observers in S' and in S will obtain rather different de Broglie wavelengths λ' and λ! Indeed,

$$\lambda' \;=\; \frac{h}{p'} \;=\; \frac{h}{p - mv} \;\neq\; \lambda, \tag{1.7}$$

This is very strange! As we review now, for ordinary waves that propagate in the rest frame of a medium (like sound waves or water waves) Galilean observers will find frequency changes but no change in wavelength. This is intuitively clear: to find the wavelength one need only take a picture of the wave at some given time, and both observers looking at the picture will agree on the value of the wavelength. On the other hand to measure frequency, each observers must wait some time to see a full period of the wave go through them. This will take different time for the different observers.

Let us demonstrate these claims quantitatively. We begin with the statement that the phase $\phi = kx - \omega t$ of such a wave is a Galilean invariant. The wave itself may be $\cos\phi$ or $\sin\phi$ or some combination, but the fact is that the physical value of the wave at any point and time must be agreed by the two observers. The wave is an observable. Since all the features of the wave (peaks, zeroes, etc, etc) are controlled by the phase, the two observers must agree on the value of the phase.

In the S frame the phase can be written as follows

$$\phi \;=\; kx - \omega t \;=\; k(x - \tfrac{\omega}{k}t) \;=\; \frac{2\pi}{\lambda}(x - Vt) \;=\; \frac{2\pi x}{\lambda} - \frac{2\pi V}{\lambda}t, \tag{1.8}$$

where $V = \frac{\omega}{k}$ is the wave velocity. Note that the wavelength is read from the coefficient of x and ω is minus the coefficient of t The two observers should agree on the value of ϕ. That is, we should have

$$\phi'(x', t') \;=\; \phi(x, t) \tag{1.9}$$

where the coordinates and times are related by a Galilean transformation. Therefore

$$\phi'(x',t') \;=\; \frac{2\pi}{\lambda}(x-Vt) \;=\; \frac{2\pi}{\lambda}(x'+vt'-Vt') = \frac{2\pi}{\lambda}x' - \frac{2\pi(V-v)}{\lambda}t'. \tag{1.10}$$

Since the right-hand side is expressed in terms of primed variables, we can read λ' from the coefficient of x' and ω' as minus the coefficient of t':

$$\lambda' = \lambda \tag{1.11}$$

$$\omega' = \frac{2\pi}{\lambda}(V-v) = \frac{2\pi V}{\lambda}\left(1-\frac{v}{V}\right) = \omega\left(1-\frac{v}{V}\right). \tag{1.12}$$

This confirms that, as we claimed, for a physical wave propagating in a medium, the wavelength is a Galilean invariant and the frequency transforms.

So what does it mean that the wavelength of matter waves change under a Galilean transformation? It means that the Ψ waves are not directly measurable! Their value does not correspond to a measurable quantity for which all Galilean observers must agree. Thus, the wavefunction need not be invariant under Galilean transformations:

$$\Psi(x,t) \;\neq\; \Psi'(x',t')\,, \tag{1.13}$$

where (x,t) and (x',t') are related by Galilean transformations and thus represent the same point and time. You will figure out in Homework the correct relation between $\Psi(x,t)$ and $\Psi'(x',t')$.

What is the frequency ω of the de Broglie wave for a particle with momentum p? We had

$$p = \hbar k \tag{1.14}$$

which fixes the wavelength in terms of the momentum. The frequency ω of the wave is determined by the relation

$$E \;=\; \hbar\omega\,, \tag{1.15}$$

which was also postulated by de Broglie and fixes ω in terms of the energy E of the particle. Note that for our focus on non-relativistic particles the energy E is determined by the momentum through the relation

$$E \;=\; \frac{p^2}{2m}\,. \tag{1.16}$$

We can give three pieces of evidence that (1.15) is a reasonable relation.

1. If we superpose matter waves to form a wave-packet that represents the particle, the packet will move with the so called group velocity v_g, which in fact coincides with the velocity of the particle. The group velocity is found by differentiation of ω with respect to k, as we will review soon:
$$v_g \;=\; \frac{d\omega}{dk} \;=\; \frac{dE}{dp} \;=\; \frac{d}{dp}\Big(\frac{p^2}{2m}\Big) \;=\; \frac{p}{m} \;=\; v\,. \tag{1.17}$$

2. The relation is also suggested by special relativity. The energy and the momentum components of a particle form a four-vector:
$$\left(\frac{E}{c}\,,\,p\right) \tag{1.18}$$

Similarly, for waves whose phases are relativistic invariant we have another four-vector

$$\left(\frac{\omega}{c}\,,\,k\right) \tag{1.19}$$

Setting two four-vectors equal to each other is a consistent choice: it would be valid in all Lorentz frames. As you can see, both de Broglie relations follow from

$$\left(\frac{E}{c}\,,\,p\right) \;=\; \hbar\left(\frac{\omega}{c}\,,\,k\right)\,. \tag{1.20}$$

3. For photons, (1.15) is consistent with Einstein's quanta of energy, because $E = h\nu \;=\; \hbar\omega$.

In summary we have

$$\boxed{p = \hbar k, \quad E = \hbar\omega\ .} \tag{1.21}$$

These are called the *de Broglie relations*, and they are valid for all particles.

2 Phase and Group Velocities

To understand group velocity we form wave packets and investigate how fast they move. For this we will simply assume that $\omega(k)$ is some arbitrary function of k. Consider a superposition of plane waves $e^{i(kx-\omega(k)t)}$ given by

$$\psi(x,t) = \int dk\ \Phi(k)e^{i(kx-\omega(k)t)}. \tag{2.22}$$

We assume that the function $\Phi(k)$ is peaked around some wavenumber $k = k_0$, as shown in Fig. 2.

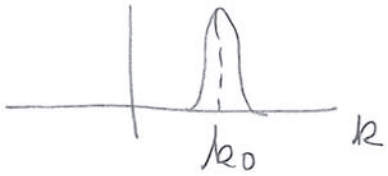

Figure 2: The function $\Phi(k)$ is assumed to peak around $k = k_0$.

In order to motivate the following discussion consider the case when $\Phi(k)$ not only peaks around k_0 but it also is *real* (we will drop this assumption later). In this case the phase φ of the integrand comes only from the exponential:

$$\varphi(k) = \;kx - \omega(k)t\,. \tag{2.23}$$

We wish to understand what are the values of x and t for which the packet $\psi(x,t)$ takes large values. We use the *stationary phase principle*: since only for $k \sim k_0$ the integral over k has a chance to give a non-zero contribution, the phase factor must be *stationary* at $k = k_0$. The idea is simple: if a function is multiplied by a rapidly varying phase, the integral washes out. Thus the phase must have zero derivative at k_0. Applying this idea to our phase we find the derivative and set it equal to zero at k_0:

$$\frac{d\varphi}{dk}\Big|_{k_0} \;=\; x - \frac{d\omega}{dk}\Big|_{k_0}\,t \;=\; 0\,. \tag{2.24}$$

This means that $\psi(x,t)$ is appreciable when x and t are related by

$$x \;=\; \frac{d\omega}{dk}\Big|_{k_0} t\,, \tag{2.25}$$

showing that the packet moves with *group velocity*

$$v_g \;=\; \frac{d\omega}{dk}\Big|_{k_0}\,. \tag{2.26}$$

Exercise. If $\Phi(k_0)$ is not real write $\Phi(k) = |\Phi(k)|e^{i\phi(k)}$. Find the new version of (2.25) and show that the velocity of the wave is not changed.

Let us now do a more detailed calculation that confirms the above analysis and gives some extra insight. Notice first that

$$\psi(x,0) \;=\; \int dk\; \Phi(k) e^{ikx}\,. \tag{2.27}$$

We expand $\omega(k)$ in a Taylor expansion around $k = k_0$

$$\omega(k) \;=\; \omega(k_0) + (k-k_0)\,\frac{d\omega}{dk}\Big|_{k_0} + \mathcal{O}\left((k-k_0)^2\right). \tag{2.28}$$

Then we find, neglecting the $\mathcal{O}((k-k_0)^2)$ terms

$$\psi(x,t) \;=\; \int dk\; \Phi(k)\, e^{ikx}\, e^{-i\omega(k_0)t} e^{-i(k-k_0)\,\frac{d\omega}{dk}\big|_{k_0} t}\,. \tag{2.29}$$

It is convenient to take out of the integral all the factors that do not depend on k:

$$\begin{aligned}\psi(x,t) &= e^{-i\omega(k_0)t + ik_0\,\frac{d\omega}{dk}\big|_{k_0} t} \int dk\; \Phi(k) e^{ikx} e^{-ik\,\frac{d\omega}{dk}\big|_{k_0} t} \\ &= e^{-i\omega(k_0)t + ik_0\,\frac{d\omega}{dk}\big|_{k_0} t} \int dk\; \Phi(k) e^{ik\left(x - \frac{d\omega}{dk}\big|_{k_0} t\right)}\,.\end{aligned} \tag{2.30}$$

Comparing with (2.27) we realize that the integral in the above expression can be written in terms of the wavefunction at zero time:

$$\psi(x,t) \;=\; e^{-i\omega(k_0)t + ik_0\,\frac{d\omega}{dk}\big|_{k_0} t}\;\; \psi\Big(x - \frac{d\omega}{dk}\Big|_{k_0} t\Big). \tag{2.31}$$

The phase factors in front of the expression are not important in tracking where the wave packet is. In particular we can take the norm of both sides of the equation to find

$$|\psi(x,t)| = \Big|\psi\Big(x - \frac{d\omega}{dk}\Big|_{k_0} t, 0\Big)\Big|. \tag{2.32}$$

If $\psi(x,0)$ peaks at some value x_0 it is clear from the above equation that $|\psi(x,t)|$ peaks for

$$x - \frac{d\omega}{dk}\Big|_{k_0} t = x_0 \quad\to\quad x \;=\; x_0 + \frac{d\omega}{dk}\Big|_{k_0} t\,, \tag{2.33}$$

showing that the peak of the packet moves with velocity $v_{\rm gr} = \frac{d\omega}{dk}$, evaluated at k_0.

3 Choosing the wavefunction for a free particle

What is the mathematical form of the wave associated with a particle a particle with energy E and momentum p? We know that ω and k are determined from $E = \hbar omega$ and $p = \hbar k$. Let's suppose that we want our wave to be propagating in the $+\hat{x}$ direction. All the following are examples of waves that could be candidates for the particle wavefunction.

1. $\sin(kx - \omega t)$
2. $\cos(kx - \omega t)$
3. $e^{i(kx-\omega t)} = e^{ikx}e^{-i\omega t}$ - time dependence $\propto e^{-i\omega t}$
4. $e^{-i(kx-\omega t)} = e^{-ikx}e^{i\omega t}$ - time dependence $\propto e^{+i\omega t}$

In the third and fourth options we have indicated that the time dependence could come with either sign. We will use superposition to decide which is the right one! We are looking for a wave-function which is non-zero for all values of x.

Let's take them one by one:

1. Starting from (1), we build a superposition in which the particle has equal probability to be found moving in the $+x$ and the $-x$ directions.

$$\Psi(x,t) = \sin(kx - \omega t) + \sin(kx + \omega t) \tag{3.1}$$

   Expanding the trigonometric functions this can be simplified to

$$\Psi(x,t) \;=\; 2\sin(kx)\cos(\omega t)\,. \tag{3.2}$$

   But this result is not sensible. The wave function vanishes identically for all x at some special times

$$\omega t = \left(\tfrac{\pi}{2}, \tfrac{3\pi}{2}, \tfrac{5\pi}{2}, ...\right) \tag{3.3}$$

   A wavefunction that is zero cannot represent a particle.

2. Constructing a wave function from (2) with a superposition of left and right going cos waves,

$$\Psi(x,t) = \cos(kx - \omega t) + \cos(kx + \omega t) = 2\cos(kx)\cos(\omega t)\,. \tag{3.4}$$

   This choice is no good, it also vanishes identically when $\omega t = \left(\tfrac{\pi}{2}, \tfrac{3\pi}{2}, ...\right)$

3. Let's try a similar superposition of exponentials from (3), with both having the same time dependence

$$\begin{aligned} \Psi(x,t) &= e^{i(kx-\omega t)} + e^{i(-kx-\omega t)} && (3.5)\\ &= (e^{ikx} + e^{-ikx})\, e^{-i\omega t} && (3.6)\\ &= 2\cos kx\, e^{-i\omega t}\,. && (3.7) \end{aligned}$$

   This wavefunction meets our criteria! It is never zero for all values of x because $e^{-i\omega t}$ is never zero.

4. A superposition of exponentials from (4) also meets our criteria

$$\begin{aligned} \Psi(x,t) &= e^{-i(kx-\omega t)} + e^{-i(-kx-\omega t)} && (3.8)\\ &= (e^{ikx} + e^{-ikx})\, e^{i\omega t} && (3.9)\\ &= 2\cos kx\, e^{i\omega t}\,. && (3.10) \end{aligned}$$

This is never zero for all values of x

Since both options (3) and (4) seem to work we ask: Can we use *both* (3) and (4) to represent a particle moving to the right (in the $+\hat{x}$ direction)? Let's assume that we can. Then, since adding a state to itself should not change the state, we could represent the right moving particle by using the sum of (3) and (4)

$$\Psi(x,t) = e^{i(kx-\omega t)} + e^{-i(kx-\omega t)} = 2\cos(kx-\omega t)\,. \tag{3.11}$$

This, however, is the same as (2), which we already showed leads to difficulties. Therefore we must choose between (3) and (4).

The choice is a matter of convention, and all physicists use the same convention. We take the free particle wavefunction to be

$$\boxed{\text{Free particle wavefunction}: \quad \Psi(x,t) \;=\; e^{i(kx-\omega t)}\,,} \tag{3.12}$$

representing a particle with

$$p = \hbar k\,, \quad \text{and} \quad E = \hbar\omega\,. \tag{3.13}$$

In three dimensions the corresponding wavefunction would be

$$\boxed{\text{Free particle wavefunction}: \quad \Psi(\mathbf{x},t) \;=\; e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\,,} \tag{3.14}$$

representing a particle with

$$\mathbf{p} = \hbar\,\mathbf{k}\,, \quad \text{and} \quad E = \hbar\omega\,. \tag{3.15}$$

Andrew Turner and Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 5

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1 Equations for a wavefunction

We determined that the wavefunction or de Broglie wave for a particle with momentum p and energy E is given by

$$\Psi(x,t) \;=\; e^{i(kx-\omega t)}\,, \tag{1.1}$$

where ω and k are determined from

$$p=\hbar k, \quad E=\hbar\omega\,, \quad E=\frac{p^2}{2m} \tag{1.2}$$

The wavefunction (1.1) represents a state of definite momentum. It is then of interest to find an operator that extracts that information from the wavefunction. The operator must be, roughly, a derivative with respect to x, as this would bring down a factor of k. In fact more precisely, we take

$$\begin{aligned}\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t) &= \frac{\hbar}{i}(ik)\Psi(x,t)\\ &= \hbar k\Psi(x,t)\\ &= p\Psi(x,t)\end{aligned} \tag{1.3}$$

where the p factor in the last right-hand side is just the momentum. We thus identify the operator $\frac{\hbar}{i}\frac{\partial}{\partial x}$ as the *momentum operator* $\hat{p}$

$$\boxed{\hat{p} \;\equiv\; \frac{\hbar}{i}\frac{\partial}{\partial x}\,.} \tag{1.4}$$

and we have verified that acting on the wavefunction $\Psi(x,t)$ for a particle of momentum p it gives p times the wavefunction:

$$\hat{p}\,\Psi \;=\; p\,\Psi\,. \tag{1.5}$$

The momentum operator it acts on wavefunctions, which are functions of space and time to give another function of x and t. Since $\hat{p}$ on Ψ gives a number (p, in fact) times Ψ we say

that Ψ is an **eigenstate** of $\hat{p}$. The matrix algebra analogy is useful: matrices are the operators and column vectors are the states. Matrices act by multiplication on column vectors. An eigenvector of a matrix is a special vector. The matrix acting on an eigenvector gives a number times the eigenvector. After the action of the matrix the direction of the vector is unchanged but its magnitude can be scaled. The same for eigenstates of operators: an operator acting on an eigenstate gives the eigenstate up to a multiplicative constant. We also say that Ψ is a state of **definite momentum**.

Let us now consider extracting the energy information from the free particle wavefunction. This time we must avail ourselves of the time derivative:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) \;=\; i\hbar(-i\omega)\Psi(x,t) \;=\; \hbar\omega\,\Psi(x,t) \;=\; E\,\Psi(x,t)\,. \tag{1.6}$$

It would seem plausible to say that the time derivative $i\hbar\frac{\partial}{\partial t}$ is an energy operator but, for a free particle the energy is given in terms of the momentum, so we can construct the relevant energy operator by working on the above right-hand side

$$E\Psi \;=\; \frac{p^2}{2m}\Psi \;=\; \frac{p}{2m}\,p\Psi \;=\; \frac{p}{2m}\,\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\,, \tag{1.7}$$

where we used equation (1.5) to write $p\Psi$ as the momentum operator acting on Ψ. Since p is a constant we can move the p factor on the last right-hand side close to the wavefuntion and then replace it by the momentum operator:

$$E\Psi \;=\; \frac{1}{2m}\,\frac{\hbar}{i}\frac{\partial}{\partial x}\,p\Psi \;=\; \frac{1}{2m}\,\frac{\hbar}{i}\frac{\partial}{\partial x}\,\frac{\hbar}{i}\frac{\partial}{\partial x}\,\Psi\,. \tag{1.8}$$

This can be written as

$$E\Psi \;=\; \frac{1}{2m}\hat{p}\,\hat{p}\,\Psi \;=\; \frac{\hat{p}^2}{2m}\,\Psi\,, \tag{1.9}$$

which suggests the following definition of the energy operator $\hat{E}$:

$$\hat{E} \;\equiv\; \frac{\hat{p}^2}{2m} \;=\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,. \tag{1.10}$$

Indeed, for our free particle wavefunction, (1.9) shows that $E\Psi = \hat{E}\Psi$.

Our work also allows us to find an differential equation for which our de Broglie wavefunction is a solution. Consider (1.6) and replace the right hand side $E\Psi$ by $\hat{E}\Psi$ giving us

$$\boxed{\;i\hbar\,\frac{\partial}{\partial t}\Psi(x,t) \;=\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)\;.\;} \tag{1.11}$$

This is the free-particle Schrödinger equation. More schematically, using the energy operator, it can be written as

$$\boxed{\;i\hbar\,\frac{\partial}{\partial t}\Psi(x,t) \;=\; \hat{E}\,\Psi(x,t)\;.\;} \tag{1.12}$$

It is worth re-checking that our de Broglie wavefunction satisfies the Schrödinger equation (1.11). Indeed for $\Psi = e^{i(kx-\omega t)}$ we find

$$i\hbar(-i\omega)\Psi \;=\; -\frac{\hbar^2}{2m}(ik)^2\Psi \tag{1.13}$$

which is a solution since the Ψ factors cancel and all that is needed is the equality

$$\hbar\omega \;=\; \frac{\hbar^2 k^2}{2m}\,, \tag{1.14}$$

which is recognized as the familiar relation $E = \frac{p^2}{2m}$.

Note that the Schrödinger equation admits more general solutions than the de Broglie wavefunction for a particle of definite momentum and definite energy. Since the equation is linear, any superposition of plane wave solutions with different values of k is a solution. Take for example

$$\Psi(x,t) \;=\; e^{i(k_1 x-\omega_1 t)} + e^{i(k_2 x-\omega_2 t)} \tag{1.15}$$

This is a solution, and note that while each summand corresponds to a state of definite momentum, the total solution is not a state of definite momentum. Indeed

$$\hat{p}\,\Psi(x,t) \;=\; \hbar k_1\; e^{i(k_1 x-\omega_1 t)} + \hbar k_2\; e^{i(k_2 x-\omega_2 t)}\,, \tag{1.16}$$

and the right hand side cannot be written as a number times Ψ. The full state is not a state of definite energy either. The general solution of the free Schrödinger equation is the most general superposition of plane waves:

$$\Psi(x,t) \;=\; \int_{-\infty}^{\infty} dk\,\Phi(k)\,e^{i(kx-\omega(k)t)}\,, \tag{1.17}$$

where $\Phi(k)$ is an *arbitrary* function of k that controls the superposition and we have written $\omega(k)$ to emphasize that ω is a function of the momentum, as in (1.14).

Exercise. Verify that Ψ in (1.17) solves the free Schrödinger equation.

We now have the tools to time-evolve any initial wavefunction. Namely, given the initial wavefunction $\Psi(x,0)$ of any packet at time equal zero, we can obtain $\Psi(x,t)$. Indeed, using Fourier transformation one can write

$$\Psi(x,0) \;=\; \int dk\,\Phi(k)\,e^{ikx}\,, \tag{1.18}$$

where $\Phi(k)$ is the Fourier transform of $\Psi(x,0)$. But then, the time evolution simply consists in adding the exponential $e^{-i\omega(k)t}$ to the integral, so that the answer for the time evolution is indeed given by (1.17).

As we have discussed before, the velocity of a wave packet described by (1.17) is given by the group velocity evaluated for the dominant value of k. We confirm that this is indeed reasonable

$$v_g \equiv \frac{\partial\omega}{\partial k} = \frac{\partial\hbar\omega}{\partial\hbar k} = \frac{\partial E}{\partial p} = \frac{\partial}{\partial p}\left(\frac{p^2}{2m}\right) = \frac{p}{m}\,, \tag{1.19}$$

which is the expected velocity for a free non-relativistic particle with momentum p and mass m.

The Schrödinger equation has an explicit i on the left-hand side. This i shows that it is impossible to find a solution for real Ψ. If Ψ were real the right-hand side of the equation would be real but the left-hand side would be imaginary. Thus, the Schrödinger equation forces us to work with complex wavefunctions.

Note also that the Schrödinger equation does not take the form of a conventional wave equation. A conventional wave equation for a variable ϕ takes the form

$$\frac{\partial^2\phi}{\partial x^2} - \frac{1}{V^2}\frac{\partial^2\phi}{\partial t^2} \;=\; 0\,. \tag{1.20}$$

The general solutions of this linear equation are $f_\pm(x \pm Vt)$. This would certainly allow for real solutions, which are not acceptable in quantum theory. The Schrödinger equation has no second-order time derivatives. It is first-order in time!

2 Schrödinger Equation for particle in a potential

Suppose now that our quantum particle is not free but rather is moving in some external potential $V(x,t)$. In this case, the total energy of the particle is no longer simply kinetic, it is the sum of kinetic and potential energies:

$$E \;=\; \frac{p^2}{2m} + V(x,t)\,, \tag{2.1}$$

This naturally suggests that the energy operator should take the form

$$\hat{E} \;=\; \frac{\hat{p}^2}{2m} + V(x,t)\,. \tag{2.2}$$

The first term, as we already know, involves second derivatives with respect to x. The second term acts multiplicatively: acting on any wavefunction $\Psi(x,t)$ it simply multiplies it by $V(x,t)$. We now postulate that the Schrödinger equation for a particle in a potential takes the form (1.12) with $\hat{E}$ replaced by the above energy operator:

$$\boxed{\;i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\Big)\Psi(x,t)\,.\;} \tag{2.3}$$

The energy operator $\hat{E}$ is usually called the **Hamiltonian** operator $\hat{H}$, so one has

$$\boxed{\;\hat{H} \equiv\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\,,\;} \tag{2.4}$$

and the Schrödinger equation takes the form

$$\boxed{\;i\hbar\frac{\partial}{\partial t}\Psi(x,t) \;=\; \hat{H}\,\Psi(x,t)\,.\;} \tag{2.5}$$

Let us reconsider the way in which the potential $V(x,t)$ is an operator. We can do this by introducing a **position** operator $\hat{x}$ that acting on functions of x gives another function of x as follows:

$$\hat{x}f(x) \;\equiv\; xf(x)\,. \tag{2.6}$$

Note that it follows from this equation and successive applications of it that

$$\hat{x}^k f(x) \;\equiv\; x^k f(x)\,. \tag{2.7}$$

If the potential $V(x,t)$ can be written as some series expansion in terms of x it then follows that

$$V(\hat{x},t)\Psi(x,t) \;\equiv\; V(x,t)\Psi(x,t)\,. \tag{2.8}$$

The operators we are dealing with (momentum, position, Hamiltonian) are all declared to be linear operators. A **linear operator** $\hat{A}$ satisfies

$$\hat{A}(a\phi) = a\,\hat{A}\phi\,, \quad \hat{A}(\phi_1+\phi_2) = \hat{A}\phi_1 + \hat{A}\phi_2\,, \tag{2.9}$$

where a is a constant. Two linear operators $\hat{A}$ and $\hat{B}$ that act on the same set of objects can always be added $(\hat{A}+\hat{B})\phi \equiv \hat{A}\phi + \hat{B}\phi$. They can also be multiplied, the product $\hat{A}\hat{B}$ is a linear operator defined by $\hat{A}\hat{B}\phi \equiv \hat{A}(\hat{B}\phi)$, meaning that you act first with $\hat{B}$, which is closest to ϕ and then act on the result with $\hat{A}$. The order of multiplication matters and thus $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ may not be the same operators. To quantify this possible difference one introduces the **commutator** $[A,B]$ of two operators, defined to be the linear operator

$$\boxed{\;[\,\hat{A}\,,\,\hat{B}\,] \;\equiv\; \hat{A}\hat{B} - \hat{B}\hat{A}\,.\;} \tag{2.10}$$

If the commutator vanishes, the two operators are said to commute. It is also clear that $[\hat{A},\hat{A}]=0$ for any operator $\hat{A}$.

We have operators $\hat{x}$ and $\hat{p}$ that are clearly somewhat related. We would like to know their commutator $[\,\hat{x}\,,\,\hat{p}\,]$. For this we let $[\,\hat{x}\,,\,\hat{p}\,]$ act on some arbitrary function $\phi(x)$ and then attempt simplification. Let's do it.

$$\begin{aligned}
[\,\hat{x}\,,\,\hat{p}\,]\phi(x) = (\hat{x}\hat{p}-\hat{p}\hat{x})\phi(x) &= \hat{x}\hat{p}\,\phi(x) - \hat{p}\hat{x}\,\phi(x) \\
&= \hat{x}(\hat{p}\phi(x)) - \hat{p}(\hat{x}\phi(x)) \\
&= \hat{x}\Big(\frac{\hbar}{i}\frac{\partial\phi(x)}{\partial x}\Big) - \hat{p}(x\phi(x)) \\
&= x\frac{\hbar}{i}\frac{\partial\phi(x)}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\phi(x)) \\
&= \frac{\hbar}{i}x\frac{\partial\phi(x)}{\partial x} - \frac{\hbar}{i}x\frac{\partial\phi(x)}{\partial x} - \frac{\hbar}{i}\phi(x) \\
&= -\frac{\hbar}{i}\phi(x) = i\hbar\,\phi(x)\,,
\end{aligned} \tag{2.11}$$

so that, all in all, we have shown that for arbitrary $\phi(x)$ one has

$$[\,\hat{x}\,,\,\hat{p}\,]\phi(x) \;=\; i\hbar\,\phi(x)\,. \tag{2.12}$$

Since this equation holds for any ϕ it really represents the equality of two operators. Whenever we have $\hat{A}\phi = \hat{B}\phi$ for arbitrary ϕ we simply say that $\hat{A} = \hat{B}$. The operators are the same because they give the same result acting on anything! We have therefore discovered the most fundamental commutation relation in quantum mechanics:

$$\boxed{[\,\hat{x}\,,\,\hat{p}\,] \;=\; i\hbar\;.} \tag{2.13}$$

The right hand side is a number, but should be viewed as an operator (acting on any function it multiplies by the number). This commutation relation can be used to prove Heisenberg's uncertainty principle, which states that the product of the position uncertainty and the momentum uncertainty must always exceed $\hbar/2$.

The idea that operators can fail to commute may remind you of matrix multiplication, which is also non-commutative. We thus have the following correspondences:

$$\begin{aligned} \text{operators} &\;\leftrightarrow\; \text{matrices} \\ \text{wavefunctions} &\;\leftrightarrow\; \text{vectors} \\ \text{eigenstates} &\;\leftrightarrow\; \text{eigenvectors} \end{aligned} \tag{2.14}$$

One can in fact formulate Quantum Mechanics using matrices, so these correspondences are actually concrete and workable.

As an example of useful matrices that do not commute, consider the Pauli matrices, three two-by-two matrices given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \;,\; \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{2.15}$$

Actually these matrices are exactly what is needed to consider spin one-half particles. The spin operator $\mathbf{S}$ has three components $S_i = \frac{\hbar}{2}\sigma_i$. Let us now see if σ_1 and σ_2 commute.

$$\begin{aligned} \sigma_1\sigma_2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \\ \sigma_2\sigma_1 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \end{aligned} \tag{2.16}$$

We then see that

$$[\sigma_1, \sigma_2] = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = 2i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 2i\sigma_3 \tag{2.17}$$

In fact, one also has $[\sigma_2, \sigma_3] = 2i\sigma_1$ and $[\sigma_3, \sigma_1] = 2i\sigma_2$.

Matrix mechanics, was worked out in 1925 by Werner Heisenberg and clarified by Max Born and Pascual Jordan. Note that, if we were to write $\hat{x}$ and $\hat{p}$ operators in matrix form, they would require infinite dimensional matrices. One can show that there are no finite size matrices that commute to give a number times the identity matrix, as is required from (2.13). This shouldn't surprise us: on the real line there are an infinite number of linearly independent wavefunctions, and in view of the correspondences in (2.14) it would suggest an infinite number of basis vectors. The relevant matrices must therefore be infinite dimensional.

Two basic properties of the Schrödinger equation

1. The differential equation is first order in time. This means that for an initial condition it suffices to know the wavefunction completely at some initial time t_0 and the Schrödinger equation then determines the wave function for all times. This can be understood very explicitly. If we know $\Psi(x, t_0)$ for all x then the right-hand side of the Schrödinger equation, which just involves x derivatives and multiplication, can be evaluated at any point x. This means that at any point x we know the time-derivative of the wavefunction (left-hand side of the Schrödinger equation) and this allows us to calculate the wavefunction a little time later.

2. Linearity and superposition. The Schrödinger equation is a linear equation for complex wavefunctions. Therefore, given two solutions Ψ_1 and Ψ_2, we can form new solutions as linear combinations $\alpha\Psi_1 + \beta\Psi_2$ with complex coefficients α and β.

We have written the Schrödinger equation for a particle on a one-dimensional potential. How about for the case of a particle in a three-dimensional potential? As we will see now, this is easily done once we realize that in three dimensions the position and momentum operators have several components! Recall that the de Broglie wavefunction

$$\Psi(\mathbf{x}, t) \;=\; e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \;=\; e^{\,i(\,k_x x+k_y y+k_z z\;-\omega t\,)} \tag{2.18}$$

corresponds to a particle carrying momentum $\mathbf{p} = \hbar\mathbf{k}$, with $\mathbf{k} = (k_x, k_y, k_z)$. Just as we did in (1.3) we can try to extract the vector momentum by using a differential operator. The relevant operator is the gradient:

$$\nabla \;=\; \Big(\frac{\partial}{\partial x}\,,\frac{\partial}{\partial y}\,,\frac{\partial}{\partial z}\Big) \tag{2.19}$$

with which we try

$$\frac{\hbar}{i}\nabla\,\Psi(x,t) = \;\frac{\hbar}{i}\left(ik_x, ik_y, ik_z\right)\Psi(x,t) \;=\; \hbar\,\mathbf{k}\,\Psi(x,t) \;=\; \mathbf{p}\,\Psi(x,t)\,. \tag{2.20}$$

We therefore define the momentum operator $\hat{\mathbf{p}}$ as follows:

$$\hat{\mathbf{p}} \;=\; \frac{\hbar}{i}\,\nabla\,. \tag{2.21}$$

If we call the momentum components $(p_1, p_2, p_3) = (p_x, p_y, p_z)$ and the coordinates as $(x_1, x_2, x_3) = (x, y, z)$ then we have that the components of the above equation are

$$\hat{p}_k \;=\; \frac{\hbar}{i}\,\frac{\partial}{\partial x_k}\,, \quad k = 1, 2, 3\,. \tag{2.22}$$

Just like we defined a position operator $\hat{x}$, we now have three position operators $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ making up $\hat{\mathbf{x}}$. With three position and three momentum operators, we now should state the nine possible commutation relations. If you recall our derivation of $[\hat{x}, \hat{p}] = i\hbar$ you will note that the commutator vanishes unless the superscripts on $\hat{x}$ and $\hat{p}$ are the same. This means that we have

$$[\,\hat{x}_i\,,\hat{p}_j\,] \;=\; i\hbar\,\delta_{ij}\,, \tag{2.23}$$

where the Kronecker delta is defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j\,, \\ 0 & \text{if } i \neq j\,. \end{cases} \tag{2.24}$$

In order to write now the general Schrödinger equation we need to consider the kinetic energy operator, or the Hamiltonian:

$$\hat{H} \;=\; \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{x},t)\,, \tag{2.25}$$

This time

$$\hat{\mathbf{p}}^2 \;=\; \hat{\mathbf{p}}\cdot\hat{\mathbf{p}} \;=\; \frac{\hbar}{i}\nabla\cdot\frac{\hbar}{i}\nabla \;=\; -\hbar^2\,\nabla^2 \tag{2.26}$$

where ∇^2 is the Laplacian operator

$$\nabla^2 \;\equiv\; \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\,. \tag{2.27}$$

The Schrödinger equation finally takes the form

$$\boxed{\; i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = \Big(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x},t)\Big)\Psi(\mathbf{x},t)\,. \;} \tag{2.28}$$

3 Interpreting the Wavefunction

Schrödinger thought that the wavefunction Ψ represents a particle that could spread out and disintegrate. The *fraction* of the particle to be found at x would be proportional to the magnitude of $|\Psi|^2$. This was problematic, as noted by Max Born (1882-1970). Born solved the Schrödinger equation for scattering of a particle in a potential, finding a wavefunction that fell like $1/r$, with r the distance to the scattering center. But Born also noticed that in the experiment one does not find fractions of particles going in many directions but rather particles remain whole. Born suggested a probabilistic interpretation. In his proposal,

> The wavefunction $\Psi(x,t)$ doesn't tell us how much of the particle is at position x at time t but rather the probability that upon measurement taken at time t we would find the particle at position x.

To make this precise we use an infinitesimal volume element with volume $d^3\mathbf{x}$ centered around some arbitrary point $\mathbf{x}$. The probability dP to find the particle within the volume element $d^3\mathbf{x}$ at time t is

$$dP \;=\; |\Psi(\mathbf{x},t)|^2\,d^3\mathbf{x}\,. \tag{3.1}$$

Consistency requires that the total probability to find the particle *somewhere* in the whole space is unity. Thus the integral of dP over all of space must give one:

$$\int_{\text{all space}} d^3\mathbf{x}\,|\Psi(\mathbf{x},t)|^2 \;=\; 1 \tag{3.2}$$

Next time we will explore the consistency of this equation with time evolution.

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Lecture 6

B. Zwiebach
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1 Normalization and time evolution

The wavefunction $\Psi(x,t)$ that describes the quantum mechanics of a particle of mass m moving in a potential $V(x,t)$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\Big)\Psi(x,t)\,, \tag{1.1}$$

or more briefly

$$i\hbar\,\frac{\partial\Psi(x,t)}{\partial t} \;=\; \hat{H}\,\Psi(x,t)\,. \tag{1.2}$$

The interpretation of the wavefunction arises by declaring that dP, defined by

$$dP \;=\; |\Psi(x,t)|^2 dx\,, \tag{1.3}$$

is the probability to find the particle in the interval dx centered on x at time t. It follows that the probabilities of finding the particle at all possible points must add up to one:

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = 1\,. \tag{1.4}$$

We will try to understand how this equation is compatible with the time evolution prescribed by the Schrödinger equation. But before that let us examine what kind of conditions are required from wavefunctions in order to satisfy (1.4).

Suppose the wavefunction has well-defined limits as $x \to \pm\infty$. If those limits are different from zero, the integral around infinity would produce an infinite result, which is inconsistent with the claim that the total integral is one. Therefore the limits should be zero:

$$\boxed{\lim_{x\to\pm\infty}\Psi(x,t) = 0\,.} \tag{1.5}$$

It is in principle possible to have a wavefunction that has no well-defined limit at infinity but is still is square integrable. But such cases do not seem to appear in practice so we will assume that (1.5) holds. It would also be natural to assume that the spatial derivative of Ψ vanishes as $x \to \pm\infty$ but, as we will see soon, it suffices to assume that the limit of the spatial derivative of Ψ is bounded

$$\boxed{\lim_{x\to\pm\infty} \frac{\partial\Psi(x,t)}{\partial x} < \infty\,.} \tag{1.6}$$

We have emphasized before that the overall numerical factor multiplying the wavefunction is not physical. But equation (1.4) seems to be in conflict with this: if a given Ψ satisfies it, the presumed equivalent 2Ψ will not! To make precise sense of probabilities it is *convenient* to work with normalized wavefunctions, but it is not necessary, as we show now. Since time plays no role in the argument, so assume in all that follows that the equations refer to some time t_0 arbitrary but fixed. Suppose you have a wavefunction such that

$$\int dx\,|\Psi|^2 \;=\; \mathcal{N} \;\neq\; 1\,. \tag{1.7}$$

Then I claim that the probability dP to find the particle in the interval dx about x is given by

$$dP \;=\; \frac{1}{\mathcal{N}}\,|\Psi|^2\,dx\,. \tag{1.8}$$

This is consistent because

$$\int dP \;=\; \frac{1}{\mathcal{N}}\int dx\,|\Psi|^2 \;=\; \frac{1}{\mathcal{N}}\cdot\mathcal{N} \;=\; 1\,. \tag{1.9}$$

Note that dP is not changed when Ψ is multiplied by any number. Thus, this picture makes it clear that the overall scale of Ψ contains no physics. As long as the integral $\int|\Psi|^2dx < \infty$ the wavefunction is said to be **normalizable, or square-integrable**. By adjusting the overall coefficient of Ψ we can then make it **normalized**. Indeed, again assuming (1.7) the new wavefunction Ψ' defined by

$$\Psi' \;=\; \frac{1}{\sqrt{\mathcal{N}}}\,\Psi\,, \tag{1.10}$$

is properly normalized. Indeed

$$\int dx|\Psi'|^2 \;=\; \frac{1}{\mathcal{N}}\int|\Psi|^2dx \;=\; 1\,. \tag{1.11}$$

We sometimes work with wavefunctions for which the integral (1.4) is infinite. Such wavefunctions can be very useful. In fact, the de Broglie plane wave $\Psi = \exp(ikx - i\omega t)$ for a free particle is a good example: since $|\Psi|^2 = 1$ the integral is in fact infinite. What this means is that $\exp(ikx - i\omega t)$ does not truly represent a single particle. To construct a square-integrable wavefunction we can use a superposition of plane waves. It is indeed a pleasant surprise that the superposition of infinitely many non-square integrable waves is square integrable!

2 The Wavefunction as a Probability Amplitude

Let's begin with a normalized wavefunction at initial time t_0

$$\int_{-\infty}^{\infty} \Psi^*(x,t_0)\Psi(x,t_0)dx = 1\,. \tag{2.1}$$

Since $\Psi(x,t_0)$ and the Schrödinger equation determine Ψ for all times, do we then have

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx \;=\; 1\;? \tag{2.2}$$

Define the **probability density** $\rho(x,t)$

$$\rho(x,t) \;\equiv\; \Psi^*(x,t)\Psi(x,t) \;=\; |\Psi(x,t)|^2\,. \tag{2.3}$$

Define also $\mathcal{N}(t)$ as the integral of the probability density throughout space:

$$\mathcal{N}(t) \;\equiv\; \int \rho(x,t)dx\,. \tag{2.4}$$

The statement in (2.1) that the wavefunction begins well normalized is

$$\mathcal{N}(t_0) = 1\,, \tag{2.5}$$

and the condition that it remain normalized for all later times is $\mathcal{N}(t) = 1$. This would be guaranteed if we showed that for all times

$$\frac{d\mathcal{N}(t)}{dt} = 0\,. \tag{2.6}$$

We call this *conservation* of probability. Let's check if the Schrödinger equation ensures this condition will hold:

$$\begin{aligned} \frac{d\mathcal{N}(t)}{dt} \;&=\; \int_{-\infty}^{\infty} \frac{\partial\rho(x,t)}{\partial t}dx \\ &=\; \int_{-\infty}^{\infty} \left(\frac{\partial\Psi^*}{\partial t}\Psi(x,t) + \Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial t}\right)dx\,. \end{aligned} \tag{2.7}$$

From the Schrödinger equation, and its complex conjugate

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \;\;\Longrightarrow\;\; \frac{\partial\Psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\Psi\,, \tag{2.8}$$

$$-i\hbar\frac{\partial\Psi^*}{\partial t} = (\hat{H}\Psi)^* \;\;\Longrightarrow\;\; \frac{\partial\Psi^*}{\partial t} = \frac{i}{\hbar}(\hat{H}\Psi)^*\,. \tag{2.9}$$

In complex conjugating the Schrödinger equation we used that the complex conjugate of the time derivative of Ψ is simply the time derivative of the complex conjugate of Ψ. To conjugate

the right hand side we simply added the star to the whole of $\hat{H}\Psi$. We now use (2.8) and (2.9) in (2.7) to find

$$\begin{aligned}\frac{d\mathcal{N}(t)}{dt} &= \int_{-\infty}^{\infty}\left(\frac{i}{\hbar}(\hat{H}\Psi)^*\,\Psi - \frac{i}{\hbar}\Psi^*(\hat{H}\Psi)\right)dx \\ &= \frac{i}{\hbar}\Big(\int_{-\infty}^{\infty}(\hat{H}\Psi)^*\,\Psi dx - \int_{-\infty}^{\infty}\Psi^*(\hat{H}\Psi)dx\Big)\,.\end{aligned} \tag{2.10}$$

To show that the time derivative of $\mathcal{N}(t)$ vanishes, it suffices to show that

$$\boxed{\int_{-\infty}^{\infty}(\hat{H}\Psi)^*\,\Psi \;=\; \int_{-\infty}^{\infty}\Psi^*(\hat{H}\Psi)\,.} \tag{2.11}$$

Equation (2.11) is the condition on the Hamiltonian operator $\hat{H}$ for conservation of probability. In fact, if $\hat{H}$ is a Hermitian operator the condition will be satisfied. The operator $\hat{H}$ is a **Hermitian** operator if it satisfies

$$\boxed{\text{Hermitian operator:}\qquad \int_{-\infty}^{\infty}(\hat{H}\Psi_1)^*\,\Psi_2 \;=\; \int_{-\infty}^{\infty}\Psi_1^*(\hat{H}\Psi_2)\,.} \tag{2.12}$$

Here we have two wavefunctions that are arbitrary, but satisfy the conditions (1.5) and (1.6). As you can see, a Hermitian operator can be switched from acting on the first function to acting on the second function. When the two functions are the same, we recover condition (2.11).

It is worth closing this circle of ideas by defining the **Hermitian conjugate** $T^\dagger$ of the linear operator T. This is done as follows:

$$\int_{-\infty}^{\infty}\Psi_1^*\,(T\Psi_2) \;=\; \int_{-\infty}^{\infty}(T^\dagger\Psi_1)^*\,\Psi_2\,. \tag{2.13}$$

The operator $T^\dagger$, which is also linear, is calculated by starting from the left-hand side and trying to recast the expression with no operator acting on the second function. An operator T is said to be Hermitian if it is equal to its Hermitian conjugate:

$$T \text{ is Hermitian if} \qquad T^\dagger = T\,. \tag{2.14}$$

Hermitian operators are very important in Quantum Mechanics. They have real eigenvalues and one can always find a basis of the state space in terms of orthonormal eigenstates. It turns out that observables in Quantum Mechanics are represented by Hermitian operators, and the possible measured values of those observables are given by their eigenvalues. Our quest to show that normalization is preserved under time evolution in Quantum Mechanics has come down to showing that the Hamiltonian operator is Hermitian.

3 The Probability Current

Let's take a closer look at the integrand of equation (2.10). Using the explicit expression for the Hamiltonian we have

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \frac{i}{\hbar}((\hat{H}\Psi)^*\,\Psi - \Psi^*(\hat{H}\Psi)) \\ &= \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\partial^2\Psi}{\partial x^2}\right) + V(x,t)\Psi^*\Psi - \Psi^*V(x,t)\Psi\right].\end{aligned} \tag{3.1}$$

The contributions from the potential cancel and we then get

$$\frac{i}{\hbar}((\hat{H}\Psi)^*\,\Psi - \Psi^*(\hat{H}\Psi)) \;=\; \frac{\hbar}{2im}\left(\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\partial^2\Psi}{\partial x^2}\right). \tag{3.2}$$

The only chance to get to show that the integral of the right-hand side is zero is to show that it is a total derivative. Indeed, it is!

$$\begin{aligned}\frac{i}{\hbar}((\hat{H}\Psi)^*\,\Psi - \Psi^*(\hat{H}\Psi)) &= \frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \\ &= -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right] \\ &= -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\,2i\,\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \\ &= -\frac{\partial}{\partial x}\left[\frac{\hbar}{m}\,\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right],\end{aligned} \tag{3.3}$$

where we used that $z - z^* = 2i\,\mathrm{Im}(z)$. Recall that the left-hand side we have evaluated is actually $\frac{\partial\rho}{\partial t}$ and therefore the result obtained so far is

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x}\left[\frac{\hbar}{m}\,\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \;=\; 0\,. \tag{3.4}$$

This equation encodes charge conservation and is of the type

$$\frac{\partial\rho}{\partial t} + \frac{\partial J}{\partial x} \;=\; 0\,, \tag{3.5}$$

where $J(x,t)$ is the current associated with the charge density ρ. We have therefore identified a probability current

$$\boxed{J(x,t) \equiv \frac{\hbar}{m}\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right).} \tag{3.6}$$

There is just one component for this current since the particle moves in one dimension. The units of J are one over time, or probability per unit time, as we now verify.

For one spatial dimension, $[\Psi] = L^{-1/2}$, which is easily seen from the requirement that $\int dx|\Psi|^2$ is unit free. (When working with d spatial dimensions the wavefunction will have units of $L^{-d/2}$). We then have

$$\left[\Psi^*\frac{\partial\Psi}{\partial x}\right] = \frac{1}{L^2}\,, \quad [\hbar] = \frac{ML^2}{T}, \quad \left[\frac{\hbar}{m}\right] = \frac{L^2}{T}\,, \tag{3.7}$$

$$\Longrightarrow\ [J] = \frac{1}{T} = \text{ probability per unit time} \tag{3.8}$$

We can now show that the time derivative of $\mathcal{N}$ is zero. Indeed, using (3.5) we have

$$\frac{d\mathcal{N}}{dt} \ = \ \int_{-\infty}^{\infty} dx\,\frac{\partial\rho}{\partial t} \ = \ -\int_{\infty}^{\infty}\frac{\partial J}{\partial x}dx \ = \ -(J(\infty,t) - J(-\infty,t))\,. \tag{3.9}$$

The derivative vanishes if the probability current vanishes at infinity. Recalling that

$$J = \frac{\hbar}{2im}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right), \tag{3.10}$$

we see that the current indeed vanishes because we restrict ourselves to wavefunctions for which $\lim_{x\to\pm\infty}\Psi = 0$ and $\lim_{x\to\pm\infty}\frac{\partial\Psi}{\partial x}$ remains bounded. We therefore have

$$\boxed{\frac{d\mathcal{N}}{dt} = 0\,,} \tag{3.11}$$

as we wanted to show.

To illustrate how probability conservation works more generally in one dimension, focus on a segment $x \in [a,b]$. Then the probability P_{ab} to find the particle in the segment $[a,b]$, is given by

$$P_{ab} = \int_a^b \rho(x,t)\,dx\,. \tag{3.12}$$

If we now take the time derivative of this and, as before, use current conservation we get

$$\frac{dP_{ab}}{dt} = -\int_a^b \frac{\partial J(x,t)}{\partial x}dt = -J(b,t) + J(a,t)\,. \tag{3.13}$$

This is the expected result. If the amount of probability in the region $[a,b]$ changes in time, it must be due to probability current flowing in or out at the edges of the interval. Assuming the currents at $x = b$ and at $x = a$ are positive, we note that probability is flowing out at $x = b$ and is coming in at $x = a$. The signs in the above right-hand side correctly reflect the effect of these flows on the rate of change of the total probability inside the segment.

4 Probability current in 3D and current conservation

The determination of the probability current $\mathbf{J}$ for a particle moving in three dimensions follows the route taken before, but we use the 3D version of the Schrödinger equation. After some work (homework) the probability density and the current are determined to be

$$\boxed{\rho(\mathbf{x},t) \;=\; |\Psi(\mathbf{x},t)|^2\,, \qquad \mathbf{J}(x,t) \;=\; \frac{\hbar}{m}\,\mathrm{Im}\,(\Psi^*\nabla\Psi)\,,} \tag{4.1}$$

and satisfy the conservation equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{J} \;=\; 0\,. \tag{4.2}$$

In three spatial dimensions, $[\Psi] = L^{-\frac{3}{2}}$ and the units of $\mathbf{J}$ are quickly determined

$$[\Psi^*\nabla\Psi] = \frac{1}{L^4}\,, \quad \left[\frac{\hbar}{m}\right] = \frac{L^2}{T} \tag{4.3}$$

$$\Longrightarrow\; [\mathbf{J}] = \frac{1}{TL^2} = \text{ probability per unit time per unit area} \tag{4.4}$$

The conservation equation (4.2) is particularly clear in integral language. Consider a fixed region V of space and the probability $Q_V(t)$ to find the particle inside the region:

$$Q_V(t) \;=\; \int_V \rho(\mathbf{x},t)d^3\mathbf{x}\,. \tag{4.5}$$

The time derivative of the probability is then calculated using the conservation equation

$$\frac{dQ_V}{dt} \;=\; \int_V \frac{\partial\rho}{\partial t}\,d^3\mathbf{x} \;=\; -\int_V \nabla\cdot\mathbf{J}\,d^3\mathbf{x}\,. \tag{4.6}$$

Finally, using Gauss' law we find

$$\frac{dQ_V}{dt} \;=\; -\int_S \mathbf{J}\cdot\mathbf{da}\,, \tag{4.7}$$

where S is the boundary of the volume V. The interpretation here is clear. The probability that the particle is inside V may change in time if there is flux of the probability current across the boundary of the region. When the volume extends throughout space, the boundary is at infinity, and the conditions on the wavefunction (which we have not discussed in the 3D case) imply that the flux across the boundary at infinity vanishes.

Our probability density, probability current, and current conservation are in perfect analogy to electromagnetic charge density, current density, and current conservation. In electromagnetism charges flow, in quantum mechanics probability flows. The terms of the correspondence are summarized by the table.

	Electromagnetism	Quantum Mechanics
ρ	charge density	probability density
Q_V	charge in a volume V	probability to find particle in V
$\mathbf{J}$	current density	probability current density

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 7

B. Zwiebach
February 28, 2016

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1 Wavepackets and Uncertainty

A wavepacket is a superposition of plane waves e^{ikx} with various wavelengths. Let us work with wavepackets at $t = 0$. Such a wavepacket is of the form

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk. \tag{1.1}$$

If we know $\Psi(x,0)$ then $\Phi(k)$ is calculable. In fact, by the Fourier inversion theorem, the function $\Phi(k)$ is the Fourier transform of $\Psi(x,0)$, so we can write

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx. \tag{1.2}$$

Note the symmetry in the two equations above. Our goal here is to understand how the uncertainties in $\Psi(x,0)$ and $\Phi(k)$ are related. In the quantum mechanical interpretation of the above equations one recalls that a plane wave with momentum $\hbar k$ is of the form e^{ikx}. Thus the Fourier representation of the wave $\Psi(x,0)$ gives the way to represent the wave as a superposition of plane waves of different momenta.

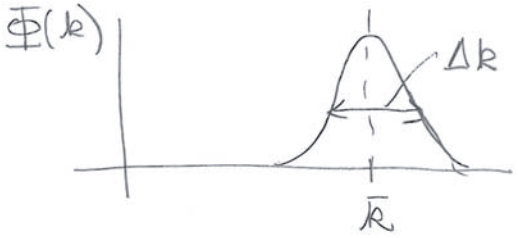

Figure 1: A $\Phi(k)$ that is centered about $k = k_0$ and has width Δk.

Let us consider a positive-definite $\Phi(k)$ that is real, symmetric about a maximum at $k = k_0$, and has a width or uncertainty Δk, as shown in Fig. 1. The resulting wavefunction $\Psi(x,0)$ is centered around $x = 0$. This follows directly from the stationary phase argument applied to (1.1). The wavefunction will have some width Δx, as shown in Fig. 2. Note that we are plotting there the absolute value $|\Psi(x,0)|$ of the wave packet. Since $\Psi(x,0)$ is complex, the other option would have been to plot the real and imaginary parts of $\Psi(x,0)$.

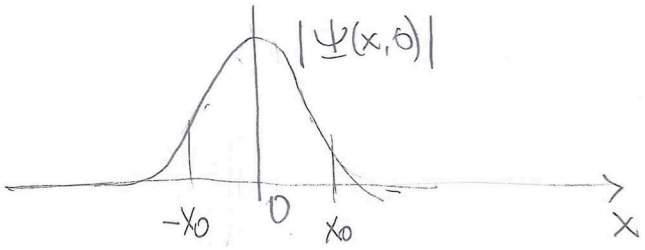

Figure 2: The $\Psi(x,0)$ corresponding to $\Phi(k)$ shown in Fig. 1, centered around $x=0$ with width Δx.

Indeed, in our case $\Psi(x,0)$ is not real! We can show that

$$\boxed{\Psi(x,0) \text{ is real if and only if } \ \Phi^*(-k)=\Phi(k)\,.} \tag{1.3}$$

Begin by complex conjugating the expression (1.1) for $\Psi(x,0)$:

$$\Psi^*(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi^*(k)e^{-ikx}dk \ =\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi^*(-k)e^{ikx}dk\,. \tag{1.4}$$

In the second step we let $k\to -k$ in the integral, which is allowable because we are integrating over *all* k, and the two sign flips, one from the measure dk and one from switching the limits of integration, cancel each other out. If $\Phi^*(-k)=\Phi(k)$ then

$$\Psi^*(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}dk=\Psi(x,0), \tag{1.5}$$

as we wanted to check. If, on the other hand we know that $\Psi(x,0)$ is real then the equality of Ψ^* and Ψ gives

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi^*(-k)e^{ikx}dk \ = \ \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}dk\,. \tag{1.6}$$

This is equivalent to

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\underbrace{\big(\Phi^*(-k)\ -\ \Phi(k)\big)}\,e^{ikx}dk \ = \ 0\,. \tag{1.7}$$

This equation actually means that the object over the brace must vanish. Indeed, the integral is computing the Fourier transform of the object with the brace, and it tells us that it is zero. But a function with zero Fourier transform must be zero itself (by the Fourier theorem). Therefore reality implies $\Phi^*(-k)=\Phi(k)$, as we wanted to show.

The condition $\Phi^*(-k)=\Phi(k)$ implies that whenever Φ is non-zero for some k it must also be non-zero for $-k$. This is not true for our chosen $\Phi(k)$: there a bump around k_0 but is no corresponding bump around $-k_0$. Therefore $\Psi(x,0)$ is not real and $\Psi(x,0)$ will have both a real and an imaginary part, both centered on $x=0$, as shown in Fig. 3.

Let's now get to the issue of width. Consider the integral for $\Psi(x,0)$

$$\Psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}dk\,, \tag{1.8}$$

and change variable of integration by letting $k=k_0+\widetilde{k}$, where the new variable of integration $\widetilde{k}$ parameterizes distance to the peak in the momentum distribution. We then have

$$\Psi(x,0)=\frac{1}{\sqrt{2\pi}}e^{ik_0x}\int_{-\infty}^{\infty}\Phi\left(k_0+\widetilde{k}\right)e^{i\widetilde{k}x}\,d\widetilde{k}. \tag{1.9}$$

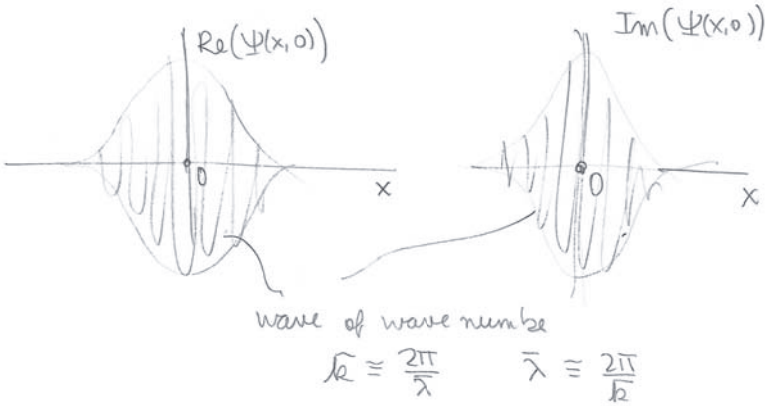

Figure 3: The real and imaginary parts of $\Psi(x,0)$.

As we integrate over $\widetilde{k}$, the most relevant region is

$$\widetilde{k} \in \left[-\tfrac{\Delta k}{2}, \tfrac{\Delta k}{2}\right] , \tag{1.10}$$

because this is where $\Phi(k)$ is large. As we sweep this region, the phase $\widetilde{k}x$ in the exponential varies in the interval

$$\widetilde{k}x \in \left[-\tfrac{\Delta k}{2}x\,,\ \tfrac{\Delta k}{2}x\right] \quad (\text{for } x>0)\,, \tag{1.11}$$

and the total phase excursion is $\Delta k\, x$. We will get a substantial contribution to the integral for a small total phase excursion; if the excursion is large, the integral will get washed out. Thus, we get a significant contribution for $\Delta k|x| \lesssim 1$, and have cancelling contributions for $\Delta k|x| \gg 1$.

From this, we conclude that $\Psi(x,0)$ will be nonzero for $x \in (-x_0, x_0)$ where x_0 is a constant for which $\Delta k x_0 \approx 1$. We identify the width of $\Psi(x,0)$ with $\Delta x := 2x_0$ and therefore we have $\Delta k\, \frac{1}{2}\Delta x \approx 1$. Since factors of two are clearly unreliable in this argument, we simply record

$$\boxed{\Delta x\, \Delta k \approx 1\,.} \tag{1.12}$$

This is what we wanted to show. The product of the uncertainty in the momentum distribution and the uncertainty in the position is a constant of order one. This uncertainty product is not quantum mechanical; as you have seen, it follows from properties of Fourier transforms.

The quantum mechanical input appears when we identify $\hbar k$ as the momentum p. This identification allows us to relate momentum and k uncertainties:

$$\Delta p \;=\; \hbar \Delta k\,. \tag{1.13}$$

As a result, we can multiply equation (1.12) by $\hbar$ to find:

$$\Delta x\, \Delta p \approx \hbar\,. \tag{1.14}$$

This is the rough version of the Heisenberg uncertainty product. The precise version requires defininining Δx and Δp precisely. One can then show that

$$\boxed{\text{Heisenberg uncertainty product:} \quad \Delta x\, \Delta p \geq \tfrac{\hbar}{2}\,.} \tag{1.15}$$

The product of uncertainties has a lower bound.

Example: Consider the case where $\Phi(k)$ is a finite step of width Δk and height $1/\sqrt{\Delta k}$, as shown in Fig. 4. Find $\Psi(x,t)$ and estimate the value of Δx.

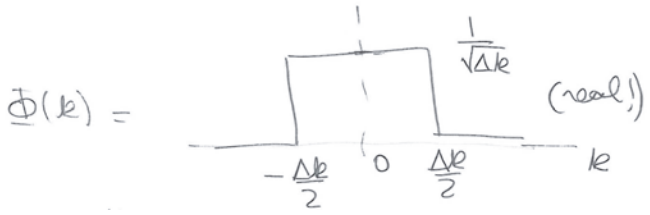

Figure 4: A momentum distribution.

Note that the $\Psi(x,0)$ we aim to calculate should be real because $\Phi^*(-k) = \Phi(k)$. From the integral representation,

$$\begin{aligned}
\Psi(x,0) &= \frac{1}{\sqrt{2\pi}} \int_{-\frac{\Delta k}{2}}^{\frac{\Delta k}{2}} \frac{1}{\sqrt{\Delta k}} e^{ikx} dk \\
&= \frac{1}{\sqrt{2\pi\Delta k}} \left. \frac{e^{ikx}}{ix} \right|_{-\frac{\Delta k}{2}}^{\frac{\Delta k}{2}} \\
&= \frac{1}{\sqrt{2\pi\Delta k}} \frac{e^{i\frac{\Delta kx}{2}} - e^{-i\frac{\Delta kx}{2}}}{ix} \\
&= \frac{1}{\sqrt{2\pi\Delta k}} \frac{2}{x} \sin\frac{\Delta kx}{2} \;=\; \sqrt{\frac{\Delta k}{2\pi}} \; \frac{\sin\frac{\Delta kx}{2}}{\frac{\Delta kx}{2}} \,.
\end{aligned} \tag{1.16}$$

We display $\Psi(x,0)$ in Fig. 5. We estimate

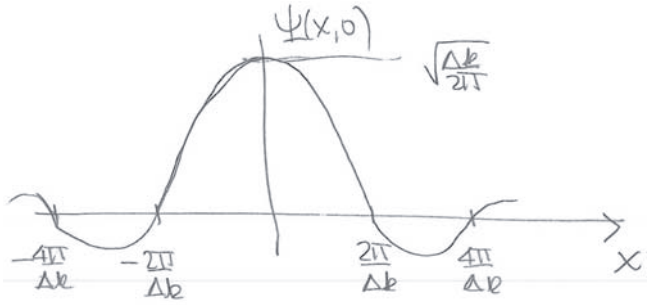

Figure 5: The $\Psi(x,0)$ corresponding to $\Phi(k)$.

$$\Delta x \approx \frac{2\pi}{\Delta k} \quad \rightarrow \quad \Delta x \Delta k \approx 2\pi \,. \tag{1.17}$$

2 Wavepacket Shape Changes

In order to appreciate general features of the motion of a wave-packet we looked at the general solution of the Schrödinger equation

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{i(kx - \omega(k)t)} dk \,, \tag{2.18}$$

and under the assumption that $\Phi(k)$ peaks around some value $k = k_0$ we expanded the frequency $\omega(k)$ in a Taylor expansion around $k = k_0$. Keeping terms up to and including $(k - k_0)^2$ we have

$$\omega(k) = \omega(k_0) + (k - k_0)\left.\frac{d\omega}{dk}\right|_{k_0} + \frac{1}{2}(k - k_0)^2\left.\frac{d^2\omega}{dk^2}\right|_{k_0} . \tag{2.19}$$

The second term played a role in the determination of the group velocity and the next term, with second derivatives of ω is responsible for the shape distorsion that occurs as time goes by. The derivatives are promptly evaluated,

$$\frac{d\omega}{dk} = \frac{dE}{dp} = \frac{p}{m} = \frac{\hbar k}{m}, \qquad \frac{d^2\omega}{dk^2} = \frac{\hbar}{m} . \tag{2.20}$$

Since all higher derivatives vanish, the expansion in (2.19) is actually exact as written. What kind of phase contribution are we neglecting when we ignore the last term in (2.19)? We have

$$e^{-i\omega(k)t} = \; e^{\cdots \; -i\frac{1}{2}(k-k_0)^2\frac{\hbar}{m}t} . \tag{2.21}$$

Assume we start with the packet at $t = 0$ and evolve in time to $t > 0$. This phase will be ignorable as long as its magnitude is significantly less than one:

$$(k - k_0)^2\frac{\hbar}{m}t \;\ll\; 1. \tag{2.22}$$

We can estimate $(k - k_0)^2 \approx (\Delta k)^2$ since the relevant k values must be within the width of the momentum distribution. Moreover since $\Delta p = \hbar\Delta k$ we get

$$\frac{(\Delta p)^2 t}{m\hbar} \;\ll\; 1. \tag{2.23}$$

Thus, the condition for minimal shape change is

$$\boxed{\; t \;\ll\; \frac{m\hbar}{(\Delta p)^2} \,.\;} \tag{2.24}$$

We can express the inequality in terms of position uncertainty using $\Delta x\Delta p \approx \hbar$. We then get

$$\boxed{\; t \;\ll\; \frac{m}{\hbar}(\Delta x)^2 \,.\;} \tag{2.25}$$

Also from (2.24) we can write

$$\frac{\Delta p\, t}{m} \;\ll\; \frac{\hbar}{\Delta p} , \tag{2.26}$$

which gives

$$\boxed{\; \frac{\Delta p}{m}\, t \;\ll\; \Delta x \,.\;} \tag{2.27}$$

This inequality has a clear interpretation. First note that $\Delta p/m$ represents the uncertainty in the velocity of the packet. There will be shape change when this velocity uncertainty through time produces position uncertainties comparable to the width Δx of the wave packet.

In all of the above inequalities we use $\ll$ and this gives the condition for *negligible* shape change. If we replace $\ll$ by $\approx$ we are giving an estimate for some *measurable* change in shape.

Exercise: Assume we have localized an electron down to $\Delta x = 10^{-10}$m. Estimate the maximum time t that it may remain localized to that level.

Using (2.25) we have

$$t \approx \frac{m(\Delta x)^2}{\hbar} = \frac{mc^2(\Delta x)^2}{\hbar c \cdot c} = \frac{0.5\,\mathrm{MeV} \cdot 10^{-20}\mathrm{m}^2}{200\,\mathrm{MeVfm} \cdot 3 \times 10^8 \mathrm{m/s}} \approx 10^{-16}\mathrm{s}. \tag{2.28}$$

If we originally had $\Delta x = 10^{-2}$m, we would have gotten $t \approx 1$s!

3 Time evolution of a free wave packet

Suppose you know the wavefunction $\Psi(x,0)$ at time equal zero. Your goal is finding $\Psi(x,t)$. This is accomplished in a few simple steps.

1. Use $\Psi(x,0)$ to compute $\Phi(k)$:

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \Psi(x,0) e^{-ikx}\,. \tag{3.1}$$

2. Use $\Phi(k)$ to rewrite $\Psi(x,0)$ as a superposition of plane waves:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk\,. \tag{3.2}$$

   This is useful because we know how plane waves evolve in time. The above is called the Fourier representation of $\Psi(x,0)$.

3. A plane wave $\psi_k(x,0) = e^{ikx}$ evolves in time into $\psi_k(x,t) = e^{i(kx-\omega(k)t)}$ with $\hbar\omega = \frac{\hbar^2 k^2}{2m}$. Using superposition we have that (3.2) evolves into

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{i(kx-\omega(k)t)} dk. \tag{3.3}$$

   This is in fact the answer for $\Psi(x,t)$. One can easily confirm this is the solution because: (i) it solves the Schrödinger equation (check that!) and (ii) setting $t = 0$ in $\Psi(x,t)$ gives us the initial wavefunction (3.2) that represented the initial condition.

4. If possible, do the integral over k to find a closed form expression for $\Psi(x,t)$. If too hard, the integral can always be done numerically.

Example: Evolution of a free Gaussian wave packet. Take

$$\psi_a(x,0) = \frac{1}{(2\pi)^{1/4}\sqrt{a}}\, e^{-x^2/4a^2}. \tag{3.4}$$

This is a gaussian wave packet at $t = 0$. The constant a has units of length and $\Delta x \approx a$. The state ψ_a is properly normalized, as you can check that $\int dx |\psi_a(x,0)|^2 = 1$.

We will not do the calculations here, but we can imagine that this packet will change shape as time evolves. What is the time scale τ for shape changes? Equation (2.25) gives us a clue. The right hand side represents a time scale for change of shape. So we must have

$$\tau \;\approx\; \frac{m}{\hbar} a^2 \,. \tag{3.5}$$

This is in fact right. You will discover when evolving the Gaussian that the relevant time interval is actually just twice the above time:

$$\tau \;\equiv\; \frac{2ma^2}{\hbar} \,. \tag{3.6}$$

If we consider the norm-squared of the wavefunction

$$|\Psi_a^*(x,0)|^2 \;=\; \frac{1}{\sqrt{2\pi}} \frac{1}{a} e^{-x^2/2a^2} \,, \tag{3.7}$$

you will find that after time evolution one has

$$|\Psi_a^*(x,t)|^2 \;=\; \frac{1}{\sqrt{2\pi}} \frac{1}{a(t)} e^{-x^2/2a^2(t)} , \tag{3.8}$$

where $a(t)$ is a time-dependent width. The goal of your calculation will be to determine $a(t)$ and to see how τ enters in $a(t)$.

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 8

B. Zwiebach
February 29, 2016

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1 Uncovering momentum space

We now begin a series of developments that lead to the idea of momentum space as a counterpoint or dual of position space. In this section the time dependence of wavefunctions will play no role. Therefore we will simply suppress time dependence. You can imagine all wavefunctions evaluated at time equal zero or at some arbitrary time t_0.

We begin by recalling the key identities of Fourier's theorem:

$$\begin{aligned} \Psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk\,, \\ \Phi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) e^{-ikx} dx\,. \end{aligned} \tag{1.1}$$

The Fourier transform $\Phi(k)$ has all the information carried by the wavefunction $\Psi(x)$. This is clear because knowing $\Phi(k)$ means knowing $\Psi(x)$. The function $\Phi(k)$ also acts as the weight with which we add the plane waves with momentum $\hbar k$ to form $\Psi(x)$.

We will now see that the consistency of the above equations can be used to derive an integral representation for a delta function. Such a representation is a needed tool for our upcoming discussion. The idea is to replace $\Phi(k)$ in the first equation by the value given in the second equation. In order to keep the notation clear, we must use x' as a dummy variable of integration in the second equation. We have

$$\begin{aligned} \Psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\; e^{ikx} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx'\; e^{-ikx'} \Psi(x') \\ &= \int_{-\infty}^{\infty} dx'\; \Psi(x')\; \underbrace{\frac{1}{2\pi} \int_{-\infty}^{\infty} dk\; e^{ik(x-x')}}\,. \end{aligned} \tag{1.2}$$

Look at the type of integral. The factor indicated by the brace happens to reduce the x' integral to an evaluation at x. We know that $\delta(x'-x)$ is the function such that for general $f(x)$,

$$\int_{-\infty}^{\infty} dx'\, f(x')\, \delta(x'-x) = f(x), \tag{1.3}$$

and so we conclude that the factor indicated by the brace is a delta function

$$\delta(x'-x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\; e^{ik(x-x')}\,. \tag{1.4}$$

In this integral one can let $k \to -k$ and since $\int dk$ is left-invariant under this replacement, we find that $\delta(x'-x) = \delta(x-x')$, or more plainly $\delta(x) = \delta(-x)$. We will record the integral representation of the delta function using the other sign:

$$\boxed{\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\; e^{ik(x-x')}\,.} \tag{1.5}$$

Another useful property of delta functions is

$$\delta(ax) = \frac{1}{|a|}\delta(x)\,. \tag{1.6}$$

At this point we ask: How does the normalization condition for $\Psi(x)$ look in terms of $\Phi(k)$? We must simply calculate. We have

$$\int_{-\infty}^{\infty} dx\; \Psi^*(x)\Psi(x) = \int_{-\infty}^{\infty} dx\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \Phi^*(k)e^{-ikx}dk\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\; \Phi(k')e^{ik'x}dk'\,. \tag{1.7}$$

Rearranging the integrals to do the x integral first we write

$$\begin{aligned}\int_{-\infty}^{\infty} dx\; \Psi^*(x)\Psi(x) =&\; \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\; \Phi^*(k)\Phi(k')\,\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{i(k'-k)x}\\ &= \int_{-\infty}^{\infty} dk\, dk'\; \Phi^*(k)\Phi(k')\delta(k'-k)\\ &= \int_{-\infty}^{\infty} dk\, \Phi^*(k)\Phi(k)\,,\end{aligned} \tag{1.8}$$

where we recognized the presence of a delta function and we did the integral over k'. Our final result is therefore

$$\boxed{\int_{-\infty}^{\infty} dx\; |\Psi(x)|^2 = \int_{-\infty}^{\infty} dk\; |\Phi(k)|^2\,.} \tag{1.9}$$

This is known as Parseval's theorem, or more generally, Plancherel's theorem. This equation relates the $\Psi(x)$ normalization to a rather analogous normalization for $\Phi(k)$. This is a hint that just like for $|\Psi(x)|^2$, we may have a probability interpretation for $|\Phi(k)|^2$.

Since physically we associate our plane waves with eigenstates of momentum, let us rewrite Parseval's theorem using momentum $p = \hbar k$. Instead of integrals over k we will have integrals over p. Letting $\widetilde{\Phi}(p) = \Phi(k)$ equations (1.1) become

$$\begin{aligned}\Psi(x) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \widetilde{\Phi}(p)e^{ipx/\hbar}dp\,,\\ \widetilde{\Phi}(p) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \Psi(x)e^{-ipx/\hbar}dx\,.\end{aligned} \tag{1.10}$$

For a more symmetric pair of equations we can redefine the function $\widetilde{\Phi}(p)$. We will let $\widetilde{\Phi}(p) \to \Phi(p)\sqrt{\hbar}$ in equations (1.10). We then obtain our final form for Fourier's relations in terms of momentum:

$$\boxed{\begin{aligned}\Psi(x) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \Phi(p)\, e^{ipx/\hbar}\, dp\,,\\ \Phi(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \Psi(x)e^{-ipx/\hbar}dx\,.\end{aligned}} \tag{1.11}$$

Similarly, Parseval's theorem (1.9) becomes

$$\boxed{\int_{-\infty}^{\infty} dx\ |\Psi(x)|^2 = \int_{-\infty}^{\infty} dp\ |\Phi(p)|^2\,.} \tag{1.12}$$

Exercise. Verify that the redefinitions we did to arrive at (1.11) indeed yield (1.12) when starting from (1.9).

Our interpretation of the top equation in (1.11) is that $\Phi(p)$ denotes the weight with which we add the momentum state $e^{ipx/\hbar}$ in the superposition that represents $\Psi(x)$. This momentum state $e^{ipx/\hbar}$ is an eigenstate of the momentum operator $\hat{p}$ with eigenvalue p. Just like we say that $\Psi(x)$ is the wavefunction in position space x, we can think of $\Phi(p)$ as the wavefunction in **momentum space** p. The Parseval identity (1.12) suggests that $\Phi(p)$ has a probabilistic interpretation as well. Given that a properly normalized $\Psi(x)$ leads to a $\Phi(p)$ that satisfies $\int dp|\Phi(p)|^2 = 1$, we postulate that:

$$\boxed{|\Phi(p)|^2 dp \text{ is the probability to find the particle with momentum in the range } (p, p+dp)\,.} \tag{1.13}$$

This makes the analogy between position and momentum space quite complete.

Let's consider the generalization to 3D. Fourier's theorem in momentum space language (namely, using $\mathbf{p}$ as opposed to $\mathbf{k}$) takes the form

$$\boxed{\begin{aligned}\Psi(\mathbf{x}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} d^3\mathbf{p}\ \Phi(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\,,\\ \Phi(\mathbf{p}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} d^3\mathbf{x}\ \Psi(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}\,.\end{aligned}} \tag{1.14}$$

Just like we did in the 1D case, if we insert the Fourier transform into the expression for $\Psi(\mathbf{x})$, we find an integral representation for the 3D δ-function

$$\begin{aligned}\Psi(\mathbf{x}) &= \frac{1}{(2\pi\hbar)^3} \int d^3\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \int d^3\mathbf{x}'\ \Psi(\mathbf{x}') e^{-i\mathbf{p}\cdot\mathbf{x}'/\hbar}\\ &= \int d^3\mathbf{x}'\ \Psi(\mathbf{x}') \frac{1}{(2\pi\hbar)^3} \int d^3\mathbf{p}\ e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')/\hbar}\\ &= \int d^3\mathbf{x}'\ \Psi(\mathbf{x}') \frac{1}{(2\pi)^3} \int d^3\mathbf{k}\ e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')},\end{aligned} \tag{1.15}$$

which leads to the identification

$$\delta^3(\mathbf{x}-\mathbf{x}') = \frac{1}{(2\pi)^3} \int d^3\mathbf{k}\ e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}. \tag{1.16}$$

It is then straightforward to derive Parseval's identity (exercise!). We find

$$\int_{-\infty}^{\infty} d^3\mathbf{x}\ |\Psi(\mathbf{x})|^2 \ = \ \int d^3\mathbf{p}\ |\Phi(\mathbf{p})|^2\,. \tag{1.17}$$

We use in 3D momentum space the same probability interpretation: $|\Phi(\mathbf{p})|^2 d^3\mathbf{p}$ is the probability to find the particle with momentum in the range $d^3\mathbf{p}$ around $\mathbf{p}$.

2 Expectation Values of Operators

Consider a random variable Q that takes values in the set $\{Q_1, \ldots, Q_n\}$ with respective probabilities $\{p_1, \ldots, p_n\}$. The *expectation value* $\langle Q \rangle$ (or *expected value*) of Q is the average value that we expect to find after repeated observation of Q, and is given by the formula

$$\langle Q \rangle = \sum_{i=1}^{n} Q_i p_i. \tag{2.18}$$

As we have seen, in a quantum system the probability for a particle to be found in $[x, x+dx]$ at time t is given by

$$\Psi^*(x,t)\Psi(x,t)\,dx. \tag{2.19}$$

Thus, the expected value of x, denoted as $\langle \hat{x} \rangle$ is given by

$$\langle \hat{x} \rangle \;\equiv\; \int_{-\infty}^{\infty} x\, \Psi^*(x,t)\Psi(x,t) dx. \tag{2.20}$$

Note that this expected value depends on t. What does $\langle \hat{x} \rangle$ correspond to physically? If we consider many copies of the physical system, and measure the position x at a time t in all of them, then the average value recorded will converge to $\langle \hat{x} \rangle$ as the number of measurements approaches infinity.

Let's discuss now the expectation value for the momentum. Since we have stated that

$$\Phi^*(p,t)\Phi(p,t)\,dp \tag{2.21}$$

is the probability to find the particle with momentum in the range $[p, p+dp]$ at time t, we define the expectation $\langle \hat{p} \rangle$ of the momentum operator as

$$\langle \hat{p} \rangle \;\equiv\; \int_{-\infty}^{\infty} p\, \Phi^*(p,t)\Phi(p,t) dp\,. \tag{2.22}$$

We will now manipulate this expression to see what form it takes in coordinate space. Using (1.11) and its complex conjugate version we have

$$\begin{aligned}
\langle \hat{p} \rangle &= \int_{-\infty}^{\infty} p\, \Phi^*(p,t)\Phi(p,t)\, dp \\
&= \int_{-\infty}^{\infty} dp\; p \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}\, \Psi^*(x,t) \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi\hbar}}\, e^{-ipx'/\hbar} \Psi(x',t) \\
&= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx\, \Psi^*(x,t) \int_{-\infty}^{\infty} dx'\; \Psi(x',t) \int_{-\infty}^{\infty} dp\; p\, e^{ipx/\hbar} e^{-ipx'/\hbar} \\
&= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx\, \Psi^*(x,t) \int_{-\infty}^{\infty} dx'\; \Psi(x',t) \int_{-\infty}^{\infty} dp\; \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) e^{ipx/\hbar} e^{-ipx'/\hbar} \\
&= \int_{-\infty}^{\infty} dx\; \Psi^*(x,t) \int_{-\infty}^{\infty} dx'\; \Psi(x',t) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp\; e^{ipx/\hbar} e^{-ipx'/\hbar}\,.
\end{aligned} \tag{2.23}$$

Letting $p = \hbar u$ in the final integral we have

$$\frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp\; e^{ipx/\hbar} e^{-ipx'/\hbar} \;=\; \frac{1}{2\pi} \int_{-\infty}^{\infty} du\; e^{iu(x-x')} \;=\; \delta(x-x')\,. \tag{2.24}$$

As a result, we have

$$\begin{aligned}\langle\hat{p}\rangle &= \int_{-\infty}^{\infty} dx\ \Psi^*(x,t)\int_{-\infty}^{\infty} dx'\ \Psi(x',t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\delta(x-x') \\ &= \int_{-\infty}^{\infty} dx\ \Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\int_{-\infty}^{\infty} dx'\ \Psi(x',t)\delta(x'-x)\,,\end{aligned} \tag{2.25}$$

where we changed the order of integration. The x' integral is now easily done and we find

$$\langle\hat{p}\rangle = \int_{-\infty}^{\infty} dx\ \Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi(x,t)\,, \tag{2.26}$$

We have thus shown that

$$\boxed{\langle\hat{p}\rangle = \int_{-\infty}^{\infty} dx\ \Psi^*(x,t)\,\hat{p}\,\Psi(x,t)\,,\quad \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}\,.} \tag{2.27}$$

Notice the position of the $\hat{p}$ operator: it acts on $\Psi(x)$. This motivates the following definition for the expectation value $\langle\hat{Q}\rangle$ of any operator $\hat{Q}$:

$$\boxed{\langle\hat{Q}\rangle = \int_{-\infty}^{\infty} dx\ \Psi^*(x,t)\,\hat{Q}\Psi(x,t)\,.} \tag{2.28}$$

Example: Consider the kinetic energy operator $\hat{T}$ for a particle moving in 1D:

$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}. \tag{2.29}$$

The definition gives

$$\langle\hat{T}\rangle = -\frac{\hbar^2}{2m}\int dx\ \Psi^*(x,t)\frac{\partial^2}{\partial x^2}\,\Psi(x,t)\,. \tag{2.30}$$

The kinetic energy is a positive operator (being proportional to the square of the momentum operator). It is therefore of interest to make this positivity manifest. Integrating by parts one of the x derivatives and ignoring boundary terms that are presumed to vanish, we find

$$\langle\hat{T}\rangle = \frac{\hbar^2}{2m}\int dx\ \left|\frac{\partial\Psi(x,t)}{\partial x}\right|^2. \tag{2.31}$$

This is manifestly positive! The expectation value of $\hat{T}$ can also be computed in momentum space using the probabilistic interpretation that led to (2.22):

$$\langle\hat{T}\rangle = \int dp\,\frac{p^2}{2m}|\Phi(p,t)|^2\,. \tag{2.32}$$

Other examples of operators whose expectation values we can now compute are the momentum operator $\hat{\mathbf{p}} \to \frac{\hbar}{i}\nabla$ in 3D, the potential energy operator, $V(\hat{\mathbf{x}})$, and the angular momentum operator

$$\begin{aligned}\hat{\mathbf{L}} &= \hat{\mathbf{r}}\times\hat{\mathbf{p}} = (\ \hat{y}\hat{p}_z - \hat{z}\hat{p}_y\ ,\ \hat{z}\hat{p}_x - \hat{x}\hat{p}_z\ ,\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x) \\ &= \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\ ,\ z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\ ,\ x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).\end{aligned} \tag{2.33}$$

3 Time dependence of expectation values

The *expectation* values of operators are in general time dependent because the wavefunctions representing the states are time dependent. We will consider here operators that do not have *explicit* time dependence, that is, operators that do no :

$$\begin{aligned} i\hbar\frac{d}{dt}\langle Q\rangle &= i\hbar\frac{d}{dt}\int_{-\infty}^{\infty} d^3x\ \Psi^*(x,t)\hat{Q}\Psi(x,t) \\ &= i\hbar\int_{-\infty}^{\infty} d^3x\ \left(\frac{\partial\Psi^*}{\partial t}\hat{Q}\Psi + \Psi^*\hat{Q}\frac{\partial\Psi}{\partial t}\right) \\ &= i\hbar\int_{-\infty}^{\infty} d^3x\ \left(\frac{i}{\hbar}(\hat{H}\Psi)^*\hat{Q}\Psi - \frac{i}{\hbar}\Psi^*\hat{Q}(\hat{H}\Psi)\right) \\ &= \int_{-\infty}^{\infty} d^3x\ \left(\Psi^*\hat{Q}\hat{H}\Psi - (\hat{H}\Psi^*)\hat{Q}\Psi\right) \end{aligned} \tag{3.34}$$

We now recall the hermiticity of $\hat{H}$, which implies that

$$\int_{-\infty}^{\infty} dx\ (\hat{H}\Psi_1)^*\Psi_2 = \int_{-\infty}^{\infty} dx\ \Psi_1^*\hat{H}\Psi_2. \tag{3.35}$$

This can be applied to the second term in the last right-hand side of (3.34) to move $\hat{H}$ into the other wavefunction

$$\begin{aligned} i\hbar\frac{d}{dt}\langle Q\rangle &= \int_{-\infty}^{\infty} d^3x\ \left(\Psi^*\hat{Q}\hat{H}\Psi - \Psi^*\hat{H}\hat{Q}\Psi\right) \\ &= \int_{-\infty}^{\infty} d^3x\ \Psi^*\left[\hat{Q},\hat{H}\right]\Psi\,, \end{aligned} \tag{3.36}$$

where we noted the appearance of the commutator. All in all, we have proven that for operators $\hat{Q}$ that do not explicitly depend on time,

$$\boxed{\ i\hbar\frac{d}{dt}\langle\hat{Q}\rangle\ =\ \left\langle\left[\hat{Q},\hat{H}\right]\right\rangle\ .\ } \tag{3.37}$$

Note that the commutator satisfies the following properties (homework):

$$[A,B] = -\,[B,A] \tag{3.38}$$

$$[A,A] = 0 \tag{3.39}$$

$$[A,B+C] = [A,B] + [A,C] \tag{3.40}$$

$$[A,BC] = [A,B]\,C + B\,[A,C] \tag{3.41}$$

$$[AB,C] = A\,[B,C] + [A,C]\,B \tag{3.42}$$

$$0 = [A,[B,C]] + [B,[C,A]] + [C,[A,B]]\,. \tag{3.43}$$

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 9

B. Zwiebach
March 3, 2016

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1 Observables and Hermitian operators

Let's begin by recalling the definition of a Hermitian operator. The operator $\hat{Q}$ is Hermitian if for the class of wavefunctions Ψ we work with,

$$\int dx\ \Psi_1^*\,\hat{Q}\Psi_2 = \int dx\ (\hat{Q}\Psi_1)^*\Psi_2\,. \tag{1.1}$$

We will sometimes use a briefer notation for the integrals of pairs of functions:

$$\boxed{(\Psi_1\,,\,\Psi_2)\ \equiv\ \int dx\,\Psi_1^*(x)\Psi_2(x)\,.} \tag{1.2}$$

Note that for any constant a

$$\big(a\Psi_1,\Psi_2\big)\ =\ a^*\big(\Psi_1,\Psi_2\big)\,,\quad \big(\Psi_1,a\Psi_2\big)\ =\ a\big(\Psi_1,\Psi_2\big)\,. \tag{1.3}$$

With this notation the condition of Hermiticity is more briefly stated

$$\hat{Q}\ \text{ is Hermitian:}\qquad \big(\Psi_1,Q\Psi_2\big)\ =\ \big(Q\Psi_1,\Psi_2\big)\,. \tag{1.4}$$

The expectation value of $\hat{Q}$ was defined by

$$\langle Q\rangle_\Psi = \int dx\ \Psi^*\,\hat{Q}\Psi\ =\ \big(\Psi\,,\,\hat{Q}\Psi\big). \tag{1.5}$$

For this formula to make sense, the state Ψ must be normalized.

Claim 1. *The expectation value of a Hermitian operator is real.* To prove this we complex conjugate the above definition. The complex conjugate of the integral is the integral of the complex conjugate of the integrand, therefore

$$\big(\langle Q\rangle_\Psi\big)^*\ =\ \int dx\ \big(\Psi^*\,\hat{Q}\Psi\big)^*\ =\int dx\ \Psi(\hat{Q}\Psi)^* = \int dx\ (\hat{Q}\Psi)^*\Psi\,. \tag{1.6}$$

Note that $\hat{Q}\Psi$ is a wavefunction, so it makes sense to take its complex conjugate (we never have to think of conjugating $\hat{Q}$). Using the Hermiticity of the operator, we move it into Ψ to get

$$\big(\langle Q\rangle_\Psi\big)^*\ =\int dx\ \Psi^*\hat{Q}\Psi = \langle Q\rangle_\Psi\,, \tag{1.7}$$

thus showing that the expectation value is indeed real.

Claim 2. *The eigenvalues of a Hermitian operator are real.* Assume the operator $\hat{Q}$ has an eigenvalue q_1 associated with a normalized eigenfunction $\psi_1(x)$:

$$\hat{Q}\psi_1(x) \;=\; q_1\psi_1(x)\,. \tag{1.8}$$

Now compute the expectation value of $\hat{Q}$ in the state ψ_1:

$$\langle\hat{Q}\rangle_{\psi_1} \;=\; (\psi_1\,,\hat{Q}\psi_1) \;=\; (\psi_1\,,q_1\,\psi_1) \;=\; q_1(\psi_1\,,\psi_1) = q_1\,. \tag{1.9}$$

By claim 1, the expectation value is real, and so is the eigenvalue q_1, as we wanted to show. Note the interesting fact that the expectation value of $\hat{Q}$ on an eigenstate is precisely given by the corresponding eigenvalue.

Consider now the collection of eigenfunctions and eigenvalues of the Hermitian operator $\hat{Q}$:

$$\hat{Q}\,\psi_1(x) = q_1\psi_1(x)\,, \tag{1.10}$$

$$\hat{Q}\,\psi_2(x) = q_2\psi_2(x)\,, \tag{1.11}$$

$$\vdots$$

The list may be finite or infinite.

Claim 3. *The eigenfunctions can be organized to satisfy orthonormality:*

$$(\psi_i,\psi_j) \;=\; \int dx\;\psi_i^*(x)\psi_j(x) = \delta_{ij}\,. \tag{1.12}$$

For $i = j$, this is just a matter of normalizing properly each eigenfunction, which we can easily do. The equation also states that different eigenfunctions are orthogonal, or have zero overlap. We now explain why this is so for $i \neq j$ with $q_i \neq q_j$. Indeed, for this we evaluate $(\psi_i,\hat{Q}\psi_j)$ in two different ways. First

$$(\psi_i,\hat{Q}\psi_j) \;=\; (\psi_i,q_j\psi_j) \;=\; q_j(\psi_i,\psi_j)\,, \tag{1.13}$$

and second, using Hermiticity of $\hat{Q}$, and the reality of the eigenvalues

$$(\psi_i,\hat{Q}\psi_j) \;=\; (\hat{Q}\psi_i,\psi_j) \;=\; (q_i\psi_i,\psi_j) \;=\; q_i(\psi_i,\psi_j)\,. \tag{1.14}$$

Equating the final right-hand sides in the two evaluations we get

$$(q_j - q_i)\,(\psi_i\,,\psi_j) \;=\; 0. \tag{1.15}$$

Since the eigenvalues were assumed different, this proves that $(\psi_i,\psi_j) = 0$, as claimed. This is not yet a full proof of (1.12) because it is possible to have **degeneracies** in the spectrum, namely, different eigenfunctions with the same eigenvalue. In that case the above argument does not work. One must then show that it is possible to choose linear combinations of the degenerate eigenfunctions that are mutually orthogonal (the orthogonality with the eigenfunctions beyond the degenerate space is automatic). This is done in 8.05!

Claim 4. *The eigenfunctions of $\hat{Q}$ for a complete set of basis functions. Any reasonable Ψ can be written as a superposition of $\hat{Q}$ eigenfunctions.* (This is the so-called spectral theorem, which is proven in 8.05 in the finite-dimensional case.) This means that

$$\boxed{\Psi(x) = \alpha_1\psi_1(x) + \alpha_2\psi_2(x) + \cdots \;=\; \sum_i \alpha_i\psi_i(x)\,,} \tag{1.16}$$

with calculable coefficients α_i. Indeed, if we know the eigenfunctions we have that α_i is calculated doing the integral of ψ_i^* against Ψ:

$$\boxed{\alpha_i \;=\; (\psi_i, \Psi)\,.} \tag{1.17}$$

We quickly prove this by doing the integral

$$\int dx\; \psi_i^*(x)\Psi(x) \;=\; \int dx\; \psi_i^*(x) \sum_j \alpha_j\psi_j(x) \;=\; \sum_j \alpha_j \int dx\; \psi_i^*(x)\psi_j(x) \;=\; \sum_j \alpha_j\delta_{ij} \;=\; \alpha_i\,. \tag{1.18}$$

The condition that Ψ is normalized implies a condition on the coefficients α_i. We have

$$\begin{aligned} \int dx\; \Psi^*(x)\Psi(x) \;&=\; \int dx\; \sum_i \alpha_i^*\psi_i^*(x) \sum_j \alpha_j\psi_j(x) \\ &=\; \sum_{i,j} \alpha_i^*\alpha_j \int dx\, \psi_i^*(x)\psi_j(x) \\ &=\; \sum_{i,j} \alpha_i^*\alpha_j\delta_{ij} \;=\; \sum_i \alpha_i^*\alpha_i\,, \end{aligned} \tag{1.19}$$

so that the normalization of Ψ implies that

$$\sum_i |\alpha_i|^2 \;=\; 1\,. \tag{1.20}$$

We are finally in the position to state the measurement postulate. This is the way in which we understand that Hermitian operators represent observables and learn the rules that they follow.

Measurement Postulate: *If we measure the Hermitian operator $\hat{Q}$ in the state Ψ, the possible outcomes for the measurement are the eigenvalues $q_1, q_2, \ldots$. The probability p_i to measure q_i is given by*

$$p_i \;=\; |\alpha_i|^2\,, \tag{1.21}$$

where $\Psi(x) = \sum_i \alpha_i\psi_i(x)$. After the outcome q_i, the state of the system becomes

$$\Psi(x) \;=\; \psi_i(x)\,. \tag{1.22}$$

This is called the collapse of the wavefunction.

The collapse of the wavefunction implies that immediately after the measurement that yielded q_i a repeated measurement of $\hat{Q}$ will yield q_i with no uncertainty. A small subtlety occurs if we have degenerate eigenstates. Suppose the wavefunction contains a piece

$$\Psi \;=\; (\alpha_i\psi_i + \alpha_k\psi_k) + \ldots \tag{1.23}$$

where ψ_i and ψ_k happen to have the same eigenvalue q and the dots represent other terms. Then if we measure q the state after the measurement collapses to the sum of those two terms

$$\Psi \;=\; \frac{\alpha_i\psi_i + \alpha_k\psi_k}{\sqrt{|\alpha_i|^2 + |\alpha_j|^2}}\,, \tag{1.24}$$

with the square root denominator included to provide the proper normalization to Ψ. As a consistency check note that the probabilities p_i to find the various eigenvalues as outcomes properly add to one:

$$\sum_i p_i \;=\; \sum_i |\alpha_i|^2 \;=\; 1\,, \tag{1.25}$$

by the normalization condition for Ψ given in (1.20). The measurement postulate follows the *Copenhagen interpretation* of quantum mechanics.

Note that the measurement postulate uses the property that any vector in a vector space can be written as a sum of different vectors in an infinite number of ways. If we are to measure $\hat{Q}_1$ we expand the state in $\hat{Q}_1$ eigenstates, if we are to measure $\hat{Q}_2$ we we expand the state in $\hat{Q}_2$ eigenstates, and so on and so forth. Each decomposition is suitable for a particular measurement. Each decomposition reveals the various probabilities for the outcomes of the specific observable.

Exercise: Use the expansion $\Psi = \sum_i \alpha_i\psi_i$ to compute the expectation value $\langle Q\rangle$. We find

$$\begin{aligned}
\langle\hat{Q}\rangle &= \int dx\; \sum_i \alpha_i^*\psi_i^*(x)\,\hat{Q}\sum_j \alpha_j\psi_j(x) \\
&= \sum_{i,j}\alpha_i^*\alpha_j \int dx\; \psi_i^*(x)\hat{Q}\psi_j(x) \\
&= \sum_{i,j}\alpha_i^*\alpha_j q_j \int dx\; \psi_i^*(x)\psi_j(x) \\
&= \sum_{i,j}\alpha_i^*\alpha_j q_j\delta_{ij} = \sum_i |\alpha_i|^2 q_i \;= \sum_i p_i q_i.
\end{aligned} \tag{1.26}$$

This matches our expectations: the expectation value of $\hat{Q}$ is the sum of the possible outcomes q_i multiplied by the corresponding probabilities p_i. This is a nice consistency check on our definition of expectation values.

Example. *Free particle on the circle* $x \in [0, L]$.
We imagine the points $x = 0$ and $x = L$ identified to form a circle of circumference L. A wavefunction $\Psi(x)$ on the circle must satisfy the periodicity condition

$$\Psi(x + L) = \Psi(x)\,, \tag{1.27}$$

Assume that at some fixed time we have the wavefunction

$$\Psi(x) \;=\; \sqrt{\frac{2}{L}}\Big(\frac{1}{\sqrt{3}}\sin\frac{2\pi x}{L} \;+\; \sqrt{\frac{2}{3}}\cos\frac{6\pi x}{L}\Big)\,. \tag{1.28}$$

This wavefunction satisfies the periodicity condition, as you should check. We want to know what are the possible values of the momentum and their corresponding probabilities.

Given our discussion, we must find the set of momentum eigenstates and rewrite the wavefunction as a superposition of such states. Momentum eigenstates are exponentials of the form e^{ikx}. Two things happen on the circle that do not happen in free space. First the momentum will be quantized as a consequence of the periodicity condition (1.27). Second, since space here is of finite length, the momentum wavefunctions will be normalizable. Consider the periodicity condition as applied to e^{ikx}. We need

$$e^{ikx} = e^{ik(x+L)} \quad \rightarrow \quad e^{ikL} = 1 \quad \rightarrow \quad kL = 2\pi m\,, \quad m \in \mathbb{Z}\,. \tag{1.29}$$

Note that m can be any integer, positive, negative, or zero. We thus write for the momentum eigenstates, labeled by m

$$\psi_m(x) \;=\; N\, e^{\frac{2\pi i m x}{L}}\,, \tag{1.30}$$

with N a real normalization constant. The normalization condition gives

$$1 \;=\; \int_0^L |\psi_m(x)|^2 dx \;=\; N^2 \int_0^L dx \;=\; N^2 L \quad \rightarrow \quad N = \frac{1}{\sqrt{L}}\,. \tag{1.31}$$

Therefore our momentum eigenstates are

$$\psi_m(x) \;=\; \frac{1}{\sqrt{L}}\, e^{\frac{2\pi i m x}{L}}\,, \tag{1.32}$$

and these are states with momentum p_m, which is calculated as follows

$$\hat{p}\,\psi_m \;=\; \frac{\hbar}{i}\frac{\partial}{\partial x}\psi_m \;=\; \frac{2\pi\, m\hbar}{L}\,\psi_m \quad \rightarrow \quad p_m \;=\; \frac{2\pi\, m\hbar}{L}\,. \tag{1.33}$$

Now that we are equipped with the momentum eigenstates we must simply rewrite the wavefunction (1.28) as a superposition of such states:

$$\Psi(x) \;=\; \sqrt{\frac{2}{3}}\frac{1}{2i}\frac{1}{\sqrt{L}}\Big(e^{\frac{2\pi i x}{L}} - e^{-\frac{2\pi i x}{L}}\Big) \;+\; \frac{2}{\sqrt{3}}\frac{1}{2}\frac{1}{\sqrt{L}}\Big(e^{\frac{6\pi i x}{L}} + e^{-\frac{6\pi i x}{L}}\Big)\,. \tag{1.34}$$

We then recognize that we have

$$\Psi(x) \;=\; \sqrt{\frac{2}{3}}\frac{1}{2i}\,\psi_1(x) - \sqrt{\frac{2}{3}}\frac{1}{2i}\,\psi_{-1}(x) + \;\frac{1}{\sqrt{3}}\,\psi_3(x) + \;\frac{1}{\sqrt{3}}\,\psi_{-3}(x)\,. \tag{1.35}$$

This is our key result: the original wavefunction written as a superposition of momentum eigenstates $\psi_m(x)$. We can now give the possible values p of the momentum and their corresponding probabilities P:

$$\begin{aligned}
p \;&=\; \;\;\frac{2\pi\hbar}{L}\,, \quad P \;=\; \Big|\sqrt{\frac{2}{3}}\frac{1}{2i}\Big|^2 \;=\; \frac{1}{6}\,,\\
p \;&=\; -\frac{2\pi\hbar}{L}\,, \quad P \;=\; \Big|-\sqrt{\frac{2}{3}}\frac{1}{2i}\Big|^2 \;=\; \frac{1}{6}\,,\\
p \;&=\; \;\;\frac{6\pi\hbar}{L}\,, \quad P \;=\; \Big|\sqrt{\frac{1}{3}}\Big|^2 \;=\; \frac{1}{3}\,,\\
p \;&=\; -\frac{6\pi\hbar}{L}\,, \quad P \;=\; \Big|\sqrt{\frac{1}{3}}\Big|^2 \;=\; \frac{1}{3}\,.
\end{aligned} \tag{1.36}$$

2 Uncertainty

For random variables, the uncertainty is the *standard deviation*—the square root of the expected value of the square of deviations from the average value. Let Q be a random variable that takes on values $Q_1, \ldots, Q_n$ with probabilities $p_1, \ldots, p_n$, respectively. The expected value is

$$\overline{Q} \;=\; \sum_i p_i Q_i \,, \tag{2.37}$$

and the variance (the square of the standard deviation) is

$$(\Delta Q)^2 \;\equiv\; \sum_i p_i (Q_i - \overline{Q})^2 \,. \tag{2.38}$$

This definition makes it clear that if $\Delta Q = 0$, then the random variable is constant: each term in the above sum must vanish, making $Q_i = \bar{Q}$, for all i. We find another useful expression by expanding the above definition

$$\begin{aligned} (\Delta Q)^2 &= \sum_i p_i Q_i^2 - 2\sum_i p_i Q_i \overline{Q} + \sum_i p_i \overline{Q}^2 \\ &= \overline{Q^2} - 2\overline{Q}\,\overline{Q} + \overline{Q}^2 = \overline{Q^2} - \overline{Q}^2 \,, \end{aligned} \tag{2.39}$$

where we used $\sum_i p_i = 1$. Therefore

$$(\Delta Q)^2 \;=\; \overline{Q^2} - \overline{Q}^2 \,. \tag{2.40}$$

Since, by definition $(\Delta Q)^2 \geq 0$, we have the interesting inequality

$$\overline{Q^2} \;\geq\; \overline{Q}^2 \,. \tag{2.41}$$

Now let us consider the quantum mechanical case. We have already defined expectation values of Hermitian operators, so we can now mimic the definition (2.40) and declare that the uncertainty $\Delta\hat{Q}_\Psi$ of an operator in a state Ψ is a real number whose square is given by

$$(\Delta Q)^2_\Psi = \langle Q^2 \rangle_\Psi - \; (\langle Q \rangle_\Psi)^2 . \tag{2.42}$$

Sometimes for brevity, we omit the label for the state,

$$\boxed{(\Delta Q)^2 = \langle Q^2 \rangle - \; \langle Q \rangle^2 \,.} \tag{2.43}$$

Claim 1. The uncertainty can also be written as the expectation value of the square of the difference between the operator and its expectation value:

$$(\Delta Q)^2 \;=\; \Big\langle \big(\hat{Q} - \langle \hat{Q} \rangle\big)^2 \Big\rangle \,. \tag{2.44}$$

Indeed, expanding the right hand side we have

$$\langle \hat{Q}^2 - 2\,\hat{Q}\langle \hat{Q} \rangle + \langle \hat{Q} \rangle^2 \rangle \;=\; \langle \hat{Q}^2 \rangle - 2\langle \hat{Q} \rangle \langle \hat{Q} \rangle + \langle \hat{Q} \rangle^2 \;=\; \langle \hat{Q}^2 \rangle \;-\; \langle \hat{Q} \rangle^2 \,. \tag{2.45}$$

Claim 2. The uncertainty can be written as the integral of the square of the norm of $(\hat{Q} - \langle \hat{Q} \rangle)\Psi$:

$$(\Delta Q)^2 \;=\; \int_{-\infty}^{\infty} dx \left| \Big(\hat{Q} - \langle Q \rangle \Big) \, \Psi(x) \right|^2 . \tag{2.46}$$

Indeed to prove this we begin with (2.44) By a very similar proof, we can show this is equivalent to

$$(\Delta Q)^2 \;=\; \Big\langle \big(\hat{Q} - \langle Q \rangle \big)^2 \Big\rangle = \int dx \; \Psi^* \Big(\hat{Q} - \langle Q \rangle \Big)^2 \Psi \, . \tag{2.47}$$

Using the Hermiticity of $\hat{Q}$ and the reality of $\langle \hat{Q} \rangle$ we can bring one of the two factors to act on Ψ^*:

$$(\Delta Q)^2 \;= \int dx \; \Big[\big(\hat{Q} - \langle Q \rangle \big) \Psi \Big]^* (Q - \langle Q \rangle) \Psi \;= \int dx \; \left| \Big(\hat{Q} - \langle Q \rangle \Big) \, \Psi \right|^2 . \tag{2.48}$$

This completes the proof of claim 2.

If $\Delta Q = 0$, then by claim 2, we must have that for all x:

$$(Q - \langle Q \rangle)\Psi(x) = 0 \, , \quad \rightarrow \quad \hat{Q}\Psi(x) = \langle \hat{Q} \rangle \Psi(x) \, . \tag{2.49}$$

We see that Ψ is an eigenstate of $\hat{Q}$, which indeed means there is no uncertainty in the measurement. Of course if Ψ is an eigenstate of $\hat{Q}$ then again $\hat{Q}\Psi = \langle \hat{Q} \rangle \Psi$ and the uncertainty vanishes. All in all, we have established the equivalence

$$\boxed{\Delta \hat{Q}_\Psi \;=\; 0 \quad \Longleftrightarrow \quad \Psi \text{ is an eigenstate of } \hat{Q} \, .} \tag{2.50}$$

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 10: Solving the Time-Independent Schrödinger Equation

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1 Stationary States

Consider the Schrödinger equation for the wavefunction $\Psi(x,t)$ with the assumption that the potential energy V is time independent:

$$i\hbar\frac{\partial\Psi}{\partial t} \;=\; \hat{H}\Psi(x,t) \;=\; \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\Psi(x,t)\,, \tag{1.1}$$

where we displayed the form of the Hamiltonian operator $\hat{H}$ with the time independent potential $V(x)$. Stationary states are a very useful class of solutions of this differential equation. The signature property of a stationary state is that the position and the time dependence of the wavefunction factorize. Namely,

$$\Psi(x\,,t) \;=\; g(t)\,\psi(x)\,, \tag{1.2}$$

for some functions g and ψ. For such a *separable* solution to exist we need the potential to be time independent, as we will see below. The solution $\Psi(x,t)$ is time-dependent but it is called stationary because of a property of observables. The expectation value of observables with no explicit time dependence in arbitrary states has time dependence. On a stationary state they do not have time dependence, as we will demonstrate.

Let us use the ansatz (1.2) for Ψ in the Schrödinger equation. We then find

$$\left(i\hbar\frac{dg(t)}{dt}\right)\psi(x) = g(t)\,\hat{H}\psi(x)\,, \tag{1.3}$$

because $g(t)$ can be moved across $\hat{H}$. We can then divide this equation by $\Psi(x,t)=g(t)\psi(x)$, giving

$$i\hbar\,\frac{1}{g(t)}\frac{dg(t)}{dt} = \frac{1}{\psi(x)}\hat{H}\psi(x)\,. \tag{1.4}$$

The left side is a function of only t, while the right side is a function of only x (a time dependent potential would have spoiled this). The only way the two sides can equal each other for all values of t and x is for both sides to be equal to a *constant* E with units of energy because $\hat{H}$ has units of energy. We therefore get two separate equations. The first reads

$$i\hbar\frac{dg}{dt} = Eg\,. \tag{1.5}$$

This is solved by

$$g(t) = e^{-iEt/\hbar}\,, \tag{1.6}$$

and the most general solution is simply a constant times the above right-hand side. From the x-dependent side of the equality we get

$$\boxed{\hat{H}\psi(x) \;=\; E\psi(x)\,.} \tag{1.7}$$

This equation is an eigenvalue equation for the Hermitian operator $\hat{H}$. We showed that the eigenvalues of Hermitian operators must be real, thus the constant E **must be real**. The equation above is called the **time-independent Schrödinger equation**. More explicitly it reads

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x)\,,} \tag{1.8}$$

Note that this equation does not determine the overall normalization of ψ. Therefore we can write the full solution without loss of generality using the $g(t)$ given above:

$$\boxed{\text{Stationary state:}\quad \Psi(x,t) = e^{-iEt/\hbar}\,\psi(x)\,,\quad \text{with}\quad E\in\mathbb{R}\;\text{ and }\hat{H}\psi = E\psi\,.} \tag{1.9}$$

Note that not only is $\psi(x)$ an eigenstate of the Hamiltonian operator $\hat{H}$, the full stationary state is also an $\hat{H}$ eigenstate

$$\hat{H}\Psi(x,t) = E\Psi(x,t)\,, \tag{1.10}$$

since the time dependent function in Ψ cancels out.

We have noted that the energy E must be real. If it was not we would also have trouble normalizing the stationary state consistently. The normalization condition for Ψ, if E is not real, would give

$$\begin{aligned} 1 \;&= \int dx\; \Psi^*(x,t)\Psi(x,t) \;= \int dx\; e^{iE^*t/\hbar}e^{-iEt/\hbar}\psi^*(x)\psi(x) \\ &= e^{i(E^*-E)t/\hbar}\int dx\;\psi^*(x)\psi(x) = e^{2\,\mathrm{Im}(E)t/\hbar}\int dx\;\psi^*(x)\psi(x). \end{aligned} \tag{1.11}$$

The final expression has a time dependence due to the exponential. On the other hand the normalization condition states that this expression must be equal to one. It follows that the exponent must be zero, i.e., E is real. Given this, we also see that the normalization condition yields

$$\boxed{\int_{-\infty}^{\infty} dx\;\psi^*(x)\psi(x) = 1\,.} \tag{1.12}$$

How do we interpret the eigenvalue E? Using (1.10) we see that the expectation value of $\hat{H}$ on the state Ψ is indeed the energy

$$\langle\hat{H}\rangle_\Psi = \int dx\;\Psi^*(x,t)\hat{H}\Psi(x,t) = \int dx\Psi^*(x,t)E\Psi(x,t) = E\int dx\Psi^*(x,t)\Psi(x,t) = E, \tag{1.13}$$

Since the stationary state is an eigenstate of $\hat{H}$, the uncertainty $\Delta\hat{H}$ of the Hamiltonian in a stationary state is zero.

There are two important observations on stationary states:

(1) The expectation value of any time-independent operator $\hat{Q}$ on a stationary state Ψ is time-independent:

$$\begin{aligned}\langle Q\rangle_{\Psi(x,t)} &= \int dx\ \Psi^*(x,t)\hat{Q}\Psi(x,t) \ = \ \int dx\ e^{iEt/\hbar}\psi^*(x)\hat{Q}e^{-iEt/\hbar}\psi(x) \\ &= \int dx\ e^{iEt/\hbar}e^{-iEt/\hbar}\psi^*(x)\hat{Q}\psi(x) = \int dx\ \psi^*(x)\hat{Q}\psi(x) \ = \ \langle Q\rangle_{\psi(x)}\,,\end{aligned} \tag{1.14}$$

since the last expectation value is manifestly time independent.

(2) The superposition of stationary states with different energies not stationary. This is clear because a stationary state requires a factorized solution of the Schrödinger equation: if we add two factorized solutions with different energies they will have different time dependence and the total state cannot be factorized. We now show that that a time-independent observable $\hat{Q}$ may have a time-dependent expectation values in such a state. Consider a superposition

$$\Psi(x,t) = c_1 e^{-iE_1 t/\hbar}\psi_1(x) + c_2 e^{-iE_2 t/\hbar}\psi_2(x), \tag{1.15}$$

where ψ_1 and ψ_2 are $\hat{H}$ eigenstates with energies E_1 and E_2, respectively. Consider a Hermitian operator $\hat{Q}$. With the system in state (1.15), its expectation value is

$$\begin{aligned}\langle Q\rangle_\Psi &= \int_{-\infty}^{\infty} dx\ \Psi^*(x,t)\hat{Q}\Psi(x,t) \\ &= \int_{-\infty}^{\infty} dx\ \left(c_1^* e^{iE_1 t/\hbar}\psi_1^*(x) + c_2^* e^{iE_2 t/\hbar}\psi_2^*(x)\right)\left(c_1 e^{-iE_1 t/\hbar}\hat{Q}\psi_1(x) + c_2 e^{-iE_2 t/\hbar}\hat{Q}\psi_2(x)\right) \\ &= \int_{-\infty}^{\infty} dx\ \left(|c_1|^2\psi_1^*\hat{Q}\psi_1 + |c_2|^2\psi_2^*\hat{Q}\psi_2 + c_1^*c_2 e^{i(E_1-E_2)t/\hbar}\psi_1^*\hat{Q}\psi_2 + c_2^*c_1 e^{-i(E_1-E_2)t/\hbar}\psi_2^*\hat{Q}\psi_1\right)\end{aligned} \tag{1.16}$$

We now see the possible time dependence arising from the cross terms. The first two terms are simple time-independent expectation values. Using the hermitically of $\hat{Q}$ in the last term we then get

$$\begin{aligned}\langle Q\rangle_\Psi = \ & |c_1|^2\langle Q\rangle_{\psi_1} + |c_2|^2\langle Q\rangle_{\psi_2} \\ & + c_1^*c_2 e^{i(E_1-E_2)t/\hbar}\int_{-\infty}^{\infty} dx\ \psi_1^*\hat{Q}\psi_2 + c_1c_2^* e^{-i(E_1-E_2)t/\hbar}\int_{-\infty}^{\infty} dx\ \psi_1(\hat{Q}\psi_2)^*\end{aligned} \tag{1.17}$$

The last two terms are complex conjugates of each other and therefore

$$\langle Q\rangle_\Psi \ = \ |c_1|^2\langle Q\rangle_{\psi_1} + |c_2|^2\langle Q\rangle_{\psi_2} \ + 2\,\mathrm{Re}\left[c_1^*c_2 e^{i(E_1-E_2)t/\hbar}\int_{-\infty}^{\infty} dx\ \psi_1^*\hat{Q}\psi_2\right]. \tag{1.18}$$

We see that this expectation value is time-dependent if $E_1 \neq E_2$ and $(\psi_1, Q\psi_2)$ is nonzero. The full expectation value $\langle Q\rangle_\Psi$ is real, as it must be for any Hermitian operator.

2 Solving for Energy Eigenstates

We will now study solutions to the time-independent Schrödinger equation

$$\hat{H}\psi(x) = E\,\psi(x). \tag{2.19}$$

For a given Hamiltonian $\hat{H}$ we are interested in finding the eigenstates ψ and the eigenvalues E, which happen to be the corresponding energies. Perhaps the most interesting feature of the above equation is that generally the value of E cannot be arbitrary. Just like finite size matrices have a set of eigenvalues, the above, time-independent Schrödinger equation may have a discrete set of possible energies. A continuous set of possible energies is also allowed and sometimes important. There are indeed many solutions for any given potential. Assuming for convenience that the eigenstates and their energies can be counted we write

$$\begin{array}{ll} \psi_1(x)\,, & E_1 \\ \psi_2(x)\,, & E_2 \\ \vdots & \vdots \end{array} \tag{2.20}$$

Our earlier discussion of Hermitian operators applies here. The energy eigenstates can be organized to form a *complete set of orthonormal functions:*

$$\int \psi_i^*(x)\psi_j(x) \;=\; \delta_{ij}\,. \tag{2.21}$$

Consider the time-independent Schrödinger equation written as

$$\frac{d^2\psi}{dx^2} \;=\; -\frac{2m}{\hbar^2}(E - V(x))\,\psi\,. \tag{2.22}$$

The solutions $\psi(x)$ depend on the properties of the potential $V(x)$. It is hard to make general statements about the wavefunction unless we restrict the types of potentials. We will certainly consider continuous potentials. We also consider potentials that are not continuous but are piece-wise continuous, that is, they have a number of discontinuities. Our potentials can easily fail to be bounded. We allow delta functions in one-dimensional potentials but do not consider powers or derivatives of delta functions. We allow for potentials that become plus infinity beyond certain points. These points represent hard walls.

We want to understand general properties of ψ and the behavior of ψ at points where the potential $V(x)$ may have discontinuities or other singularities. We claim: **we must have a continuous wavefunction**. If ψ is discontinuous then ψ' contains delta-functions and ψ'' in the above left-hand side contains derivatives of delta functions. This would require the right-hand side to have derivatives of delta functions, and those would have to appear in the potential. Since we have declared that our potentials contain no derivatives of delta functions we must indeed have a continuous ψ.

Consider now four possibilities concerning the potential:

(1) $V(x)$ is continuous. In this case the continuity of $\psi(x)$ and (2.22) imply ψ'' is also continuous. This requires ψ' continuous.

(2) $V(x)$ has finite discontinuities. In this case ψ'' has finite discontinuities: it includes the product of a continuous ψ against a discontinuous V. But then ψ' must be continuous, with non-continuous derivative.

(3) $V(x)$ contains delta functions. In this case ψ'' also contains delta functions: it is proportional to the product of a continuous ψ and a delta function in V. Thus ψ' has finite discontinuities.

(4) $V(x)$ contains a hard wall. A potential that is finite immediately to the left of $x = a$ and becomes infinite for $x > a$ is said to have a hard wall at $x = a$. In such a case, the wavefunction will vanish for $x \geq a$. The slope ψ' will be finite as $x \to a$ from the left, and will vanish for $x > a$. Thus ψ' is discontinuous at the wall.

In the first two cases ψ' is continuous, and in the second two it can have a finite discontinuity. In conclusion

Both ψ and ψ' are continuous unless the potential has delta functions or hard walls in which cases ψ' may have finite discontinuities.	(2.23)

Let us give an slightly different argument for the continuity of ψ and $\frac{d\psi}{dx}$ in the case of a potential with a finite discontinuity, such as the step shown in Fig. 1.

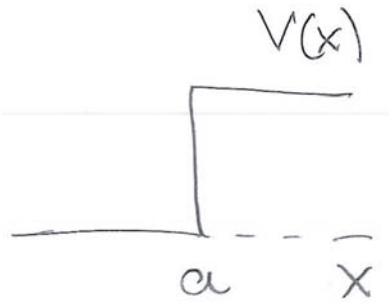

Figure 1: A potential $V(x)$ with a finite discontinuity at $x = a$.

Integrate both sides of (2.22) $a - \epsilon$ to $a + \epsilon$, and then take $\epsilon \to 0$. We find

$$\int_{a-\epsilon}^{a+\epsilon} dx \, \frac{d}{dx}\left(\frac{d\psi}{dx}\right) \;=\; -\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx \, (E - V(x))\psi(x)\,. \tag{2.24}$$

The left-hand side integrand is a total derivative so we have

$$\left.\frac{d\psi}{dx}\right|_{a+\epsilon} - \left.\frac{d\psi}{dx}\right|_{a-\epsilon} \;=\; \frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx \, (V(x) - E)\psi(x)\,. \tag{2.25}$$

By definition, the discontinuity in the derivative of ψ at $x = a$ is the limit as $\epsilon \to 0$ of the left-hand side:

$$\Delta_a\left(\frac{d\psi}{dx}\right) \;\equiv\; \lim_{\epsilon\to 0}\left(\left.\frac{d\psi}{dx}\right|_{a+\epsilon} - \left.\frac{d\psi}{dx}\right|_{a-\epsilon}\right). \tag{2.26}$$

Back in (2.25) we then have

$$\Delta_a\left(\frac{d\psi}{dx}\right) \;=\; \lim_{\epsilon\to 0}\;\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx \, (V(x) - E)\psi(x)\,. \tag{2.27}$$

The potential V is discontinuous but not infinite around $x = a$, nor is ψ infinite around $x = a$ and, of course, E is assumed finite. As the integral range becomes vanishingly small about $x = a$ the integrand remains finite and the integral goes to zero. We thus have

$$\Delta_a\left(\frac{d\psi}{dx}\right) = 0\,. \tag{2.28}$$

There is no discontinuity in $\frac{d\psi}{dx}$. This gives us one of our boundary conditions.

To learn about the continuity of ψ we reconsider the first integral of the differential equation. The integration that led to (2.25) now applied to the range from $x_0 < a$ to x yields

$$\frac{d\psi(x)}{dx} \;=\; \frac{d\psi}{dx}\Big|_{x_0} - \frac{2m}{\hbar}\int_{x_0}^{x}(E - V(x'))dx'. \tag{2.29}$$

Note that the integral on the right is a bounded function of x. We now integrate again from $a-\epsilon$ to $a+\epsilon$. Since the first term on the right-hand side is a constant we find

$$\psi(a+\epsilon) - \psi(a-\epsilon) = 2\epsilon\,\frac{d\psi}{dx}\Big|_{x_0} - \frac{2m}{\hbar}\int_{a-\epsilon}^{a+\epsilon}dx\int_{x_0}^{x}dx'\,(E - V(x')). \tag{2.30}$$

Taking the $\epsilon \to 0$ limit, the first term on the right-hand side clearly vanishes and the second term goes to zero because $\int_{x_0}^{x} dx'\,(E - V(x'))$ is a bounded function of x. As a result we have

$$\Delta_a\psi = 0\,, \tag{2.31}$$

showing that the wavefunction is continuous at $x = a$. This is our second boundary condition.

3 Free particle on a circle.

Consider now the problem of a particle confined to a circle of circumference L. The coordinate along the circle is called x and we can view the circle as the interval $x \in [0, L]$ with the endpoints identified. It is perhaps clearer mathematically to think of the circle as the full real line x with the identification

$$x \sim x + L\,, \tag{3.1}$$

which means that two points whose coordinates are related in this way are to be considered **the same point**. If follows that we have the periodicity condition

$$\psi(x + L) = \psi(x)\,. \tag{3.2}$$

From this it follows that not only ψ is periodic but all of its derivatives are also periodic.

The particle is assumed to be free and therefore $V(x) = 0$. The time-independent Schrödinger equation is then

$$-\frac{\hbar^2}{2m}\,\frac{d^2\psi}{dx^2} \;=\; E\,\psi(x)\,. \tag{3.3}$$

Before we solve this, let us show that any solution must have $E \geq 0$. For this multiply the above equation by $\psi^*(x)$ and integrate over the circle $x \in [0\,, L)$. Since ψ is normalized we get

$$-\frac{\hbar^2}{2m}\int_0^L \psi^*(x)\frac{d^2\psi}{dx^2}\,dx \;=\; E\int \psi^*(x)\psi(x)dx = E\,. \tag{3.4}$$

The integrand on the left hand side can be rewritten as

$$-\frac{\hbar^2}{2m}\int_0^L \Big[\frac{d}{dx}\Big(\psi^*\frac{d\psi}{dx}\Big) - \frac{d\psi^*}{dx}\frac{d\psi}{dx}\Big]\,dx \;=\; E\,. \tag{3.5}$$

and the total derivative can be integrated

$$-\frac{\hbar^2}{2m}\Big[\Big(\psi^*\frac{d\psi}{dx}\Big)\Big|_{x=L}-\Big(\psi^*\frac{d\psi}{dx}\Big)\Big|_{x=0}\Big]+\frac{\hbar^2}{2m}\int_0^L\Big|\frac{d\psi}{dx}\Big|^2dx \;=\; E\,. \tag{3.6}$$

Since $\psi(x)$ and its derivatives are periodic, the contributions from $x=L$ and $x=0$ cancel out and we are left with

$$E \;=\; \frac{\hbar^2}{2m}\int_0^L\Big|\frac{d\psi}{dx}\Big|^2dx\geq 0\,, \tag{3.7}$$

which establishes our claim. We also see that $E=0$ requires ψ constant (and nonzero!).

Having shown that all solutions must have $E\geq 0$ let us go back to the Schrödinger equation, which can be rewritten as

$$\frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\,\psi\,. \tag{3.8}$$

We can then define k via

$$k^2 \;\equiv\; \frac{2mE}{\hbar}\geq 0\,. \tag{3.9}$$

Since $E\geq 0$, the constant k is real. Note that this definition is very natural, since it makes

$$E=\frac{\hbar^2k^2}{2m}\,, \tag{3.10}$$

which means that, as usual, $p=\hbar k$. Using k^2 the differential equation becomes the familiar

$$\frac{d^2\psi}{dx^2}=-k^2\psi\,. \tag{3.11}$$

We could write the general solution in terms of sines and cosines of kx, but let's use complex exponentials:

$$\psi(x)\sim e^{ikx}. \tag{3.12}$$

This solves the differential equation and, moreover, it is a momentum eigenstate. The periodicity condition (3.2) requires

$$e^{ik(x+L)}=e^{ikx}\quad\rightarrow\quad e^{ikL}=1\quad\rightarrow\quad kL=2\pi n\,,\quad n\in\mathbb{Z}\,. \tag{3.13}$$

We see that momentum is quantized because the wavenumber is quantized! The wavenumber has discrete possible values

$$k_n \;\equiv\; \frac{2\pi n}{L}\,,\qquad n\in\mathbb{Z}. \tag{3.14}$$

All integers positive and negative are allowed and are in fact necessary because they all correspond to *different* values of the momentum $p_n=\hbar k_n$. The solutions to the Schrödinger equation can then be indexed by the integer n:

$$\psi_n(x)=Ne^{ik_nx}\,, \tag{3.15}$$

where N is a real normalization constant. Its value is determined from

$$1=\int_0^L\psi_n^*(x)\psi_n(x)dx=\int_0^L N^2dx \;=\; N^2L\quad\rightarrow\quad N=\frac{1}{\sqrt{L}}\,, \tag{3.16}$$

so we have

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x} = \frac{1}{\sqrt{L}} e^{\frac{2\pi i n x}{L}}\,.} \tag{3.17}$$

The associated energies are

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 4\pi^2 n^2}{2mL^2} = \frac{2\pi^2\hbar^2 n^2}{mL^2}. \tag{3.18}$$

There are infinitely many energy eigenstates. We have degenerate states because E_n is just a function of $|n|$ and thus the same for n and $-n$. Indeed ψ_n and ψ_{-n} both have energy E_n. The only nondegenerate eigenstate is $\psi_0 = \frac{1}{\sqrt{L}}$, which is a constant wavefunction with zero energy.

Whenever we find degenerate energy eigenstates we must wonder what makes those states different, given that they have the same energy. To answer this one must find an observable that takes different values on the states. Happily, in our case we know the answer. Our degenerate states can be distinguished by their momentum: ψ_n has momentum $2\pi n\frac{\hbar}{L}$ and ψ_{-n} has momentum $(-2\pi n\frac{\hbar}{L})$.

Given two degenerate energy eigenstates, any linear combination of these states is an eigenstate with the same energy. Indeed if

$$\hat{H}\psi_1 = E\psi_1\,, \quad \hat{H}\psi_2 = E\psi_2\,, \tag{3.19}$$

then

$$\hat{H}(a\psi_1 + b\psi_2) \;=\; a\hat{H}\psi_1 + b\hat{H}\psi_2 \;=\; aE\psi_1 + bE\psi_2 \;=\; E(a\psi_1 + b\psi_2)\,. \tag{3.20}$$

We can therefore form two linear combinations of the degenerate eigenstates ψ_n and ψ_{-n} to obtain another description of the energy eigenstates:

$$\begin{aligned} \psi_n + \psi_{-n} &\sim \cos(k_n x)\,, \\ \psi_n - \psi_{-n} &\sim \sin(k_n x)\,. \end{aligned} \tag{3.21}$$

While these are real energy eigenstates, they are not momentum eigenstates. Only our exponentials are simultaneous eigenstates of both $\hat{H}$ and $\hat{p}$.

The energy eigenstates ψ_n are automatically orthonormal since they are $\hat{p}$ eigenstates with no degeneracies (and as you recall eigenstates of a hermitian operator with different eigenvalues are automatically orthogonal) :

$$\int_0^L \psi_n^*(x)\psi_m(x)dx = \frac{1}{L}\int_0^L e^{\frac{2\pi i(m-n)x}{L}}dx \;=\; \delta_{mn}. \tag{3.22}$$

They are also complete: we can then construct a general wavefunction as a superposition that is in fact a Fourier series. For any $\Psi(x,0)$ that satisfies the periodicity condition, we can write

$$\Psi(x,0) = \sum_{n\in\mathbb{Z}} a_n\,\psi_n(x), \tag{3.23}$$

where, as you should check, the coefficients a_n are determined by the integrals

$$a_n = \int_0^L dx\,\psi_n^*(x)\,\Psi(x,0)\,. \tag{3.24}$$

The initial state $\Psi(x,0)$ is then easily evolved in time:

$$\Psi(x,t) = \sum_{n\in\mathbb{Z}} a_n\,\psi_n(x)e^{-\frac{iE_n t}{\hbar}}. \tag{3.25}$$

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 11

B. Zwiebach
March 17, 2016

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1 The Infinite Square Well

In our last lecture we examined the quantum wavefunction of a particle moving in a circle. Here we introduce another instructive toy model, the **infinite square well potential**. This forces a particle to live on an interval of the real line, the interval conventionally chosen to be $x \in [0, a]$. At the ends 0 and a of the interval there are hard walls that prevent the particle from going to $x > a$ and $x < 0$. The potential is defined as follows and shown in figure 1.

$$V(x) \;=\; \begin{cases} 0\,, & 0 < x < a\,, \\ \infty & x \leq 0\,,\, x \geq 0 \end{cases} \tag{1.1}$$

It is reasonable to assume that the wavefunction must vanish in the region where the potential is

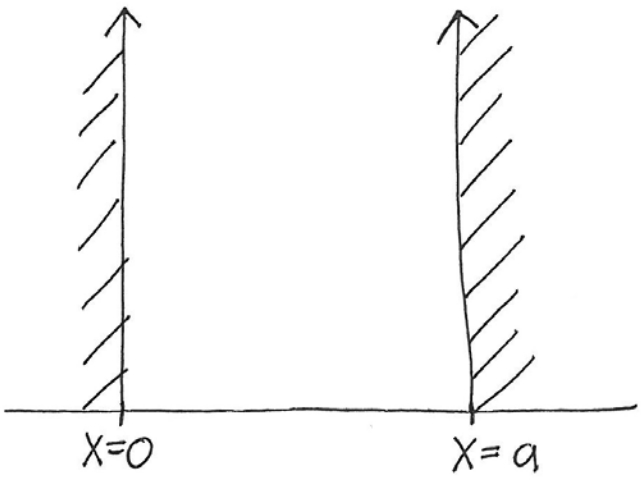

Figure 1: The infinite square well potential

infinite. Classically any region where the potential exceeds the energy of the particle is forbidden. Not so in quantum mechanics. But even in quantum mechanics a particle can't be in a region of *infinite* potential. We will be able to justify these claims by studying the more complicated *finite* square well in the limit as the height of the potential goes to infinity. But for the meantime we simply state the fact:

$$\psi(x) = 0 \quad \text{for } \; x < 0 \text{ and for } \; x > a\,. \tag{1.2}$$

Since the wavefunction must be continuous we must have that it should vanish at $x = 0$ and at $x = a$:

1. $\psi(x=0)=0$.

2. $\psi(x=a)=0$.

These are our boundary conditions. You may wonder about the continuity of the first derivative $\psi'(x)$. This derivative vanishes outside the interval and continuity would say that ψ' should vanish at 0 and at a. But this is impossible. A solution of Schrödinger's equation (a second order differential equation) for which *both* the wavefunction and its derivative vanishes at a point is identically zero! If a solution exist we must accept that ψ' can have discontinuities at an infinite wall. Therefore we do not impose any boundary condition on ψ'. The two conditions above will suffice to find a solution. In that solution ψ' is discontinuous at the endpoints.

In the region $x \in [0,a]$ the potential vanishes and the Schrödinger equation takes the form

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi\,, \tag{1.3}$$

and as we did before, one can show that the energy E must be positive (do it!). This allows us to define, as usual, a real quantity k such that

$$k^2 \;\equiv\; \frac{2mE}{\hbar^2} \quad\to\quad E \;=\; \frac{\hbar^2k^2}{2m}\,. \tag{1.4}$$

The differential equation is then

$$\frac{d^2\psi}{dx^2} \;=\; -k^2\psi\,, \tag{1.5}$$

and the general solution can be written as

$$\psi(x) \;=\; c_1\cos kx + c_2\sin kx\,, \tag{1.6}$$

with constants c_1 and c_2 to be determined. For this we use our boundary conditions.

The condition $\psi(x=0)=0$ implies that c_1 in Eq 1.6 must be zero. The coefficient of $\sin kx$ need not be, since this function vanishes automatically for $x=0$. Therefore the solution so far reads

$$\psi(x) \;=\; c_2\sin kx\,. \tag{1.7}$$

Note that if we demanded continuity of ψ' we would have to ask for $\psi'(x=0)=0$ and that would make c_2 equal to zero, and thus ψ identically zero. That **is not** a solution. There is no particle if $\psi=0$.

At this point we must impose the vanishing of ψ at $x=a$.

$$c_2\sin ka \;=\; 0 \quad\to\quad ka \;=\; n\pi \quad\to\quad k_n \;=\; \frac{n\pi}{a}\,. \tag{1.8}$$

Here n must be an integer and the solution would be

$$\psi_n(x) \;=\; N\sin\Big(\frac{n\pi x}{a}\Big)\,, \tag{1.9}$$

with N a normalization constant. Which integers n are acceptable here? Well, $n=0$ is not acceptable, because it would make the wavefunction zero. Moreover, n and $-n$ give the same wavefunction, up to a sign. Since the sign of a wavefunction is irrelevant, it would thus be double counting to include both positive and negative n's. We restrict ourselves to n being positive integers.

To solve for the coefficient, we utilize the normalization condition; every $\psi_n(x)$ must be normalized.

$$1 = N^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx \;=\; N^2\, \tfrac{1}{2} \cdot a \quad \rightarrow \quad N \;=\; \sqrt{\frac{2}{a}}\,. \tag{1.10}$$

Therefore, all in all, our solutions are:

$$\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin\Big(\frac{n\pi x}{a}\Big)\,, \quad E_n \;=\; \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2}\,, \quad n = 1, 2, \cdots .} \tag{1.11}$$

Each value of n gives a different energy, implying that in the one-dimensional infinite square well there are no degeneracies in the energy spectrum! The ground state –the lowest energy state– corresponds to $n = 1$ and has nonzero energy.

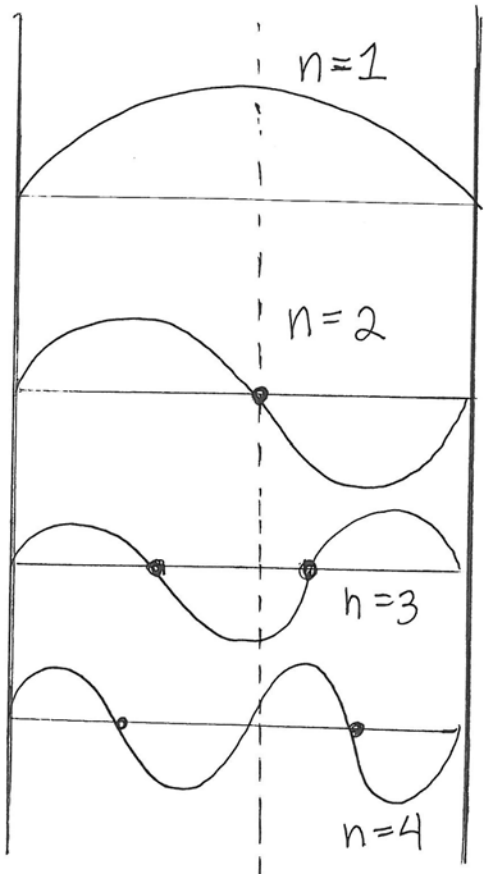

Figure 2: The four lowest energy eigenstates for the infinite square well potential. The n^{th} wavefunction solution ψ_n has $n-1$ nodes. The solutions are alternately symmetric and antisymmetric about the midpoint $x = a$.

Figure 2 shows the first four solutions to the 1-d infinite square well, labeled from $n = 1$ to $n = 4$. We note a few features:

1. The ground state $n = 1$ has no nodes. A node is a zero of the wavefunction that is not at the ends of the domain of the wavefunction. The zeroes at $x = 0$ and $x = a$ do not count as nodes. Clearly $\psi_1(x)$ does not vanish anywhere in the interior of $[0, a]$ and therefore it has no nodes. It

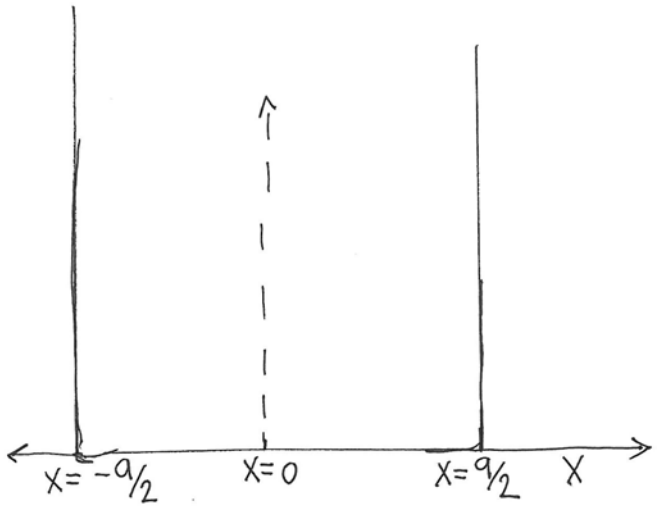

Figure 3: The infinite square well shifted to the left to make it symmetric about the origin.

is in fact true that any normalizable ground state of a one-dimensional potential does not have nodes.

2. The first excited state, $n = 2$ has one node. It is at $x = a$, the midpoint of the interval. The second excited state, $n = 3$ has two nodes. The pattern in fact continues. The n-th excited state will have n nodes.

3. In the figure the dotted vertical line marks the interval midpoint $x = \frac{a}{2}$. We note that the ground state is symmetric under reflection about $x = \frac{a}{2}$. The first excited state is antisymmetric, indeed its node is at $x = \frac{a}{2}$. The second excited state is again symmetric. Symmetry and antisymmetry alternate forever.

4. The symmetry just noted is not accidental. It holds, in general for potentials $V(x)$ that are even functions of x: $V(-x) = V(x)$. Our potential, does not satisfy this equation, but this could have been changed easily and with no consequence. We could shift the well over so that rather than having $V(x) = 0$ from $0 \leq x \leq a$, it extends from $-\frac{a}{2} \leq x \leq \frac{a}{2}$ and then it would be symmetric about the origin $x = 0$ (see figure 3). We will later prove that the bound states of a one-dimensional even potential are either even or odd! Here we are just seeing an example of such result.

5. The wavefunctions $\psi_n(x)$ with $n = 1, 2, \ldots$ form a complete set that can be used to expand any function in the interval $x \in [0, a]$ that vanishes at the endpoints. If the function does not vanish at the endpoints, the convergence of the expansion is delicate, and physically such wavefunction would be problematic as one can verify that the expectation value of the energy is infinite.

2 The Finite Square Well

We now examine the finite square well, defined as follows and shown in figure 4.

$$V(x) = \begin{cases} -V_0\,, & \text{for} \quad |x| \leq a\,, \quad V_0 > 0\,, \\ 0\,, & \text{for} \quad |x| \geq a\,. \end{cases} \tag{2.12}$$

Note that the potential energy is zero for $|x| > a$. The potential energy is negative and equal to $-V_0$ in the well, because we defined V_0 to be a positive number. The width of the well is $2a$. Note

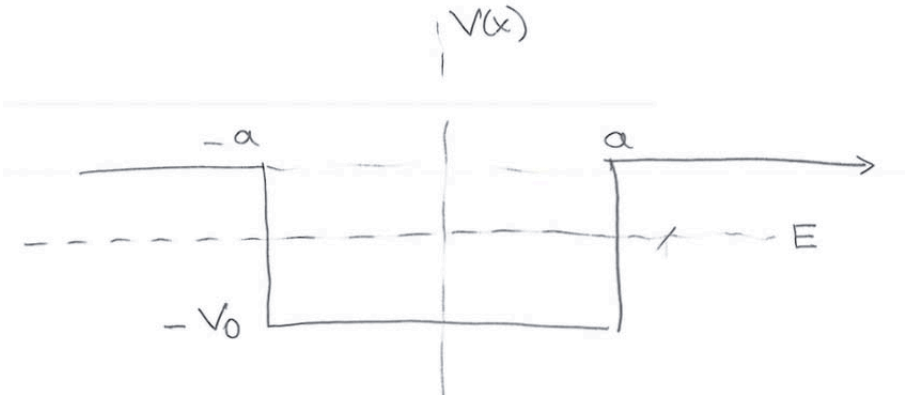

Figure 4: The finite square well potential

also that we have placed the bottom of the well differently than in the case of the infinite square well. The bottom of the infinite square well was at zero potential energy. If we wanted to obtain the infinite square well as a limit of the finite square well we would have to take V_0 to infinity, but care is needed to compare energies. The ones in the infinite square well are measured with respect to a bottom at zero energy. The ones in the finite square well are measure with respect to a bottom at $-V_0$.

We will be interested in **bound states** namely, energy eigenstates that are normalizable. For this the energy E of the states must be negative. This is readily understood. If $E > 0$, any solutions in the region $x > a$ where the potential vanishes would be a plane wave, extending all the way to infinity. Such a solution would not be normalizable. The energy E is shown as a dashed line in the figure. We have

$$-V_0 < E < 0\,. \tag{2.13}$$

Note that since E is negative we have $E = -|E|$. For a bound state of energy E, the energy $\tilde{E}$ measured with respect to the bottom of the potential is

$$\tilde{E} \;=\; E - (-V_0) = V_0 - |E| > 0\,. \tag{2.14}$$

Those $\tilde{E}$ are the ones that can be compared with the energies of the infinite square well in the limit as $V_0 \to \infty$.

What are the bound state solutions to the Schrödinger equation with this potential? We have to examine how the equation looks in the various regions where the potential is constant and then use boundary conditions to match the solutions across the points where the potential is discontinuous. We have the equation Let's examine the regions, where, for simplicity, we define $A(x)$ by

$$\frac{d^2\psi}{dx^2} = \; -\frac{2m}{\hbar^2}(E - V(x))\,\psi = \alpha(x)\psi\,, \tag{2.15}$$

where we have defined the factor $\alpha(x)$ that multiplies the wavefunction on the right-hand side of the Schrödinger equation. We then consider the two regions

- region $|x| > a$: $\alpha(x)$ is a positive constant. The wavefunction in this region constructed with real exponentials.

- region $|x| < a$: $\alpha(x)$ is a negative constant. The wavefunction in this region is constructed with trigonometric functions.

The potential $V(x)$ for the finite square well is an even function of x: $V(-x) = V(x)$ We can therefore use the theorem cited earlier (and proven later!) that for an even potential the bound states are either symmetric or antisymmetric. We begin by looking for even solutions, that is, solutions ψ for which $\psi(-x) = \psi(x)$.

Even solutions. Since the potential is piecewise continuous we must study the differential equation in two regions:

- $|x| < a$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E-(-V_0))\psi = -\frac{2m}{\hbar^2}(V_0-|E|)\psi \tag{2.16}$$

$V_0 - |E|$ is a positive constant thus define a real $k > 0$ by

$$\boxed{k^2 \equiv \frac{2m}{\hbar^2}(V_0-|E|) > 0\,, \quad k > 0\,.} \tag{2.17}$$

It is interesting to note that this equation is not too different from the free-particle equation $k^2 = \frac{2mE}{\hbar^2}$. Indeed, $V_0 - |E|$ is the kinetic energy of the particle and thus k has the usual interpretation. The differential equation to be solved now reads

$$\psi'' = -k^2\psi\,, \tag{2.18}$$

for which the only possible even solution is

$$\boxed{\psi(x) = \cos kx\,, \quad |x| < a\,.} \tag{2.19}$$

We are not including a normalization constant because, at this state we do not aim for normalized eigenstates. We will get an eigenstate and while it will not be normalized, it will be *normalizable*, and that's all that is essential. We are after is the possible energies. Normalized wavefunctions would be useful to compute expectation values.

- $|x| > a$

$$\psi'' = -\frac{2m}{\hbar^2}(E-0)\,\psi = \frac{2m|E|}{\hbar^2}\,\psi \tag{2.20}$$

This time we define a real positive constant κ with the relation

$$\boxed{\kappa^2 = \frac{2m|E|}{\hbar^2}\,, \quad \kappa > 0\,.} \tag{2.21}$$

The differential equation to be solved now reads

$$\psi'' = \kappa^2\psi\,, \tag{2.22}$$

and the solutions are exponentials. In fact we need exponentials that decay as $x \to \pm\infty$, otherwise the wavefunction will not be normalizable. This should be physically intuitive, in a

classically forbidden region the probability to be far away from the well must be vanishingly small. For $x > a$ we choose the decaying exponential

$$\boxed{\psi(x) = A\, e^{-\kappa x},\ \ x > a\,,} \tag{2.23}$$

where A is a normalization constant to be determined by the boundary conditions. More generally, given that the solution is even, we have

$$\psi(x) \ = \ A\, e^{-\kappa|x|},\ |x| > a\,. \tag{2.24}$$

It is now useful to note that κ^2 and k^2 satisfy a simple relation. Using their definitions above we see that the energy $|E|$ drops out of their sum and we have

$$k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2} \tag{2.25}$$

At this point we make progress by introducing **unit free** constants ξ, η, and z_0 as follows:

$$\begin{aligned} \eta \ &\equiv \ ka > 0\,, \\ \xi \ &\equiv \ \kappa a > 0\,, \\ z_0^2 \ &\equiv \ \frac{2mV_0a^2}{\hbar^2}\,. \end{aligned} \tag{2.26}$$

Clearly ξ is a proxy for κ and η is a proxy for k. Both depend on the energy of the bound state. The parameter z_0, unit-free, just depends on the data associated with the potential (the depth V_0 and the width $2a$) and the mass m of the particle. If you are given a potential, you know the number z_0. A very deep and/or wide potential has very large z_0, while a very shallow and/or narrow potential has small z_0. As we will see the value of z_0 tells us how many bound states the square well has.

Multiplying (2.25) by a^2 and using our definitions above we get

$$\boxed{\eta^2 + \xi^2 \ = \ z_0^2\,.} \tag{2.27}$$

Let us make clear that solving for ξ is actually like solving for the energy. From Eq. (2.21), we can see

$$\xi^2 \ = \ \kappa^2 a^2 \ = \ \frac{2m|E|a^2}{\hbar^2} \ = \ \frac{2mV_0a^2}{\hbar^2}\frac{|E|}{V_0} \ = \ z_0^2\frac{|E|}{V_0}\,, \tag{2.28}$$

and from this we get

$$\frac{|E|}{V_0} \ = \ \Big(\frac{\xi}{z_0}\Big)^2. \tag{2.29}$$

This is a nice equation, the left hand side gives the energy as a fraction of the depth V_0 of the well and the right-hand side involves ξ and the constant z_0 of the potential. The quantity η also encodes the energy in a slightly different way. From (2.17) we have

$$\eta^2 \ = \ k^2a^2 \ \equiv \ \frac{2ma^2}{\hbar^2}(V_0 - |E|)\,, \tag{2.30}$$

and using (2.14) we see that this provides the energy $\tilde{E}$, measured relative to the bottom of the potential

$$\tilde{E} \;=\; V_0 - |E| \;=\; \eta^2 \frac{\hbar^2}{2ma^2}\,. \tag{2.31}$$

This formula is convenient to understand how the infinite square energy levels appear in the limit as the depth of the finite well goes to infinity. Note that the above answer for the energies is given by the unit free number η multiplied by the characteristic energy of an infinite well of width a.

Let us finally complete the construction. We must impose the continuity of the wavefunction and the continuity of ψ' at $x = a$. Using the expressions for ψ for $x < a$ and for $x > a$ these conditions give

$$\begin{aligned} \psi \text{ continuous at } x = a \implies \qquad \cos(ka) &= Ae^{-\kappa a} \\ \psi' \text{ continuous at } x = a \implies \quad -k\sin(ka) &= -\kappa A e^{-\kappa a}\,, \end{aligned} \tag{2.32}$$

Dividing the second equation by the first we eliminate the constant A and find a second relation between k and κ! This is exactly what is needed. The result is

$$k\tan ka \;= \kappa \quad \to \quad ka\tan ka \;= \kappa a \quad \to \quad \xi = \eta\tan\eta\,. \tag{2.33}$$

Our task of finding the bound states is now reduced to finding solutions to the simultaneous equations

$$\boxed{\text{Even solutions: } \eta^2 + \xi^2 \;=\; z_0^2\,, \quad \xi = \eta\tan\eta\,, \quad \xi\,,\eta > 0\,.} \tag{2.34}$$

These equations can be solved numerically to find all solutions that exist for a given fixed value of z_0. Each solution represents one bound state. We can understand the solution space by plotting these two equations in the *first quadrant* of an (η, ξ) plane, as shown in figure 5.

The first equation in (2.34) is a piece of a circle of radius z_0. The second equation, $\xi = \eta\tan\eta$, gives infinitely many curves as η grows from zero to infinity. The value of ξ goes to infinity for η approaches each odd multiple of $\pi/2$. The bound states are represented by the intersections in the plot (heavy dots).

In the figure we see two intersections, which means two bound states. The first intersection takes place near $\eta = \pi/2$ and with large $\xi \sim z_0$. This is the ground state, or the most deeply bound bound-state. This can be seen from (2.29). Alternatively, it can be seen from equation (2.31), noting that this is the solution with smallest η. The second solution occurs for η near $3\pi/2$. As the radius of the circle becomes bigger we get more and more intersections; z_0 controls the number of even bound states. Finally, note that there is always an even solution, no matter how small z_0 is, because the arc of the circle will always intersect the first curve of the $\xi = \eta\tan\eta$ plot. Thus, at least one bound state exists however shallow the finite well is.

Odd solutions. For odd solutions all of our definitions $(k, \kappa, z_0, \eta, \xi)$ remain the same. The wavefunction now is of the form

$$\psi(x) \;=\; \begin{cases} \sin kx\,, & |x| < a \\ Ae^{-k|x|}\,, & |x| > a \end{cases} \tag{2.35}$$

Matching ψ and ψ' at $x = a$ now gives $\xi = -\eta\cot\eta$ (do it!). As a result the relevant simultaneous equations are now

$$\boxed{\text{Odd solutions:} \quad \eta^2 + \xi^2 \;= z_0^2\,, \quad \xi = -\eta\cot\eta\,, \quad \xi\,,\eta > 0\,.} \tag{2.36}$$

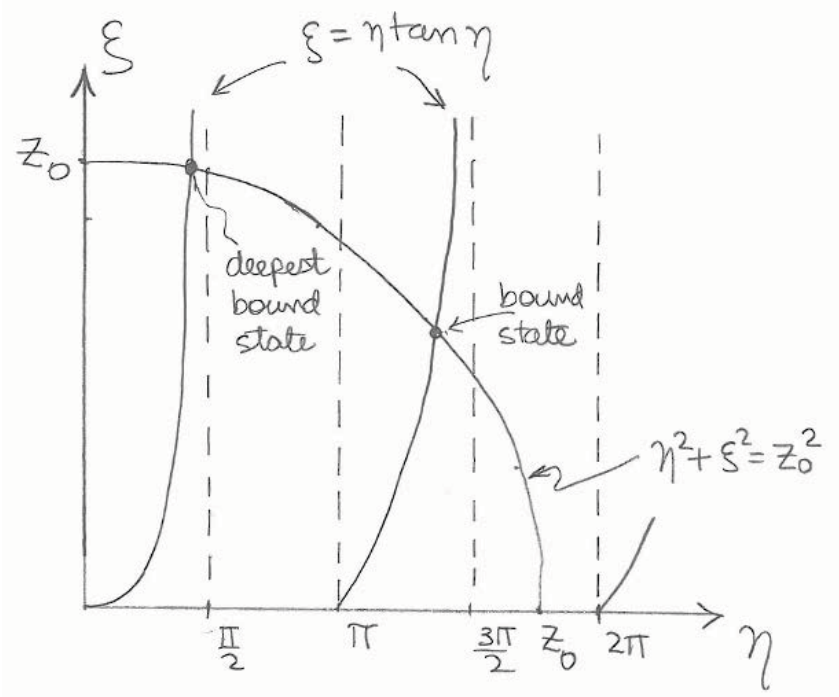

Figure 5: Graphical representation of the simultaneous equations (2.34). The intersections of the circle with the $\eta \tan \eta$ function represent even bound state solutions in the finite square well potential. The deepest bound state is the one with lowest η.

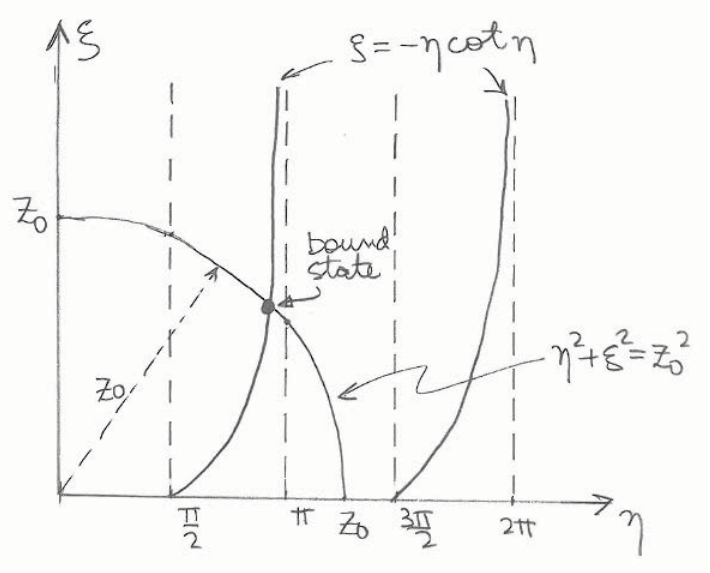

Figure 6: Graphical representation of (2.36). The intersections of the circle with the curves $\xi = -\eta \cot \eta$ are odd bound-state solutions in the finite square-well potential. In the case displayed there is just one bound state.

In figure 6 the curve $\xi = -\eta \cot \eta$ does not appear for $\eta < \pi/2$ because ξ is then negative. For $z_0 < \frac{\pi}{2}$ there are no odd bound-state solutions, but we still have the even bound state.

We could have anticipated the quantization of the energy by the following argument. Suppose you

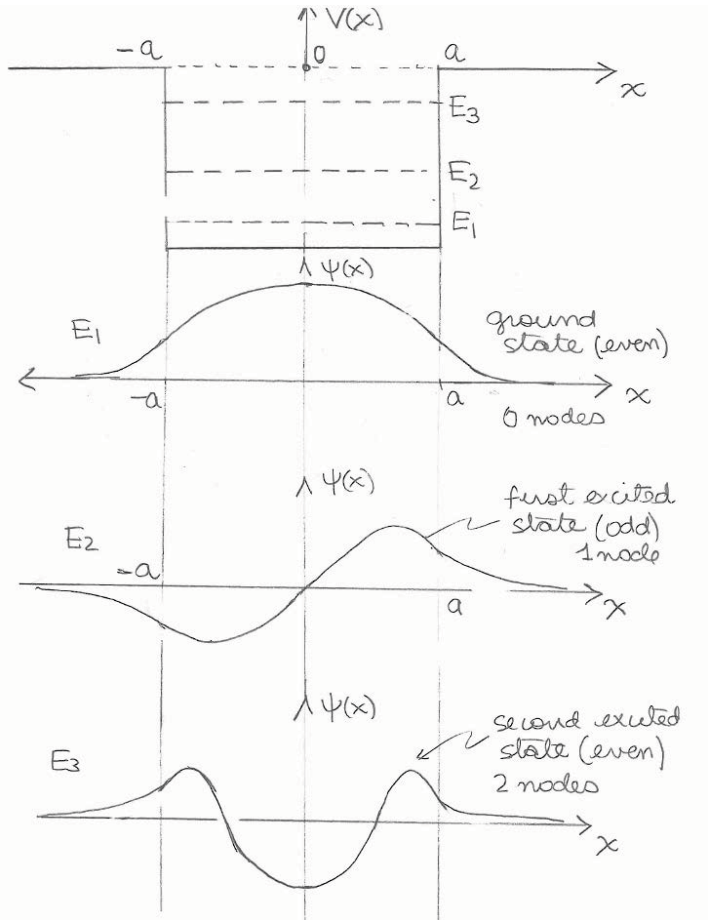

Figure 7: Sketching eigenstates of a finite square well potential. The energies are $E_1 < E_2 < E_3$.

try to calculate energy eigenstates which, as far as solving the Schrödinger equation, are determined up to an overall normalization. Suppose you don't know the energy is quantized and you fix some arbitrary fixed energy and calculate. Both in the even and in the odd case, we can set the coefficient of the $\sin kx$ or $\cos kx$ function inside the well equal to one. The coefficient of the decaying exponential outside the well was undetermined, we called it A. Therefore we just have one unknown, A. But we have two equations, because we impose continuity of ψ and of ψ' at $x = a$. If we have one unknown and two equations, we have no reason to believe there is a solution. Indeed, generally there is none. But then, if we think of the energy E as an unknown, that energy appears at various places in the equations (in k and κ) and therefore having two unknowns A and E and two equations, we should expect a single solution! This is indeed what happened.

In figure 7 we sketch the energy eigenstates of a square-well potential with three bound states of energies $E_1 < E_2 < E_3$. A few features of the wavefunctions are manifest: they alternate as even, odd, and even. They have zero, one, and two nodes, respectively. The second derivative of ψ is negative for $|x| < a$ and positive for $|x| > a$ (it is in fact discontinuous at $x = \pm a$). The exponential decay in the region $|x| > a$ is fastest for the ground state and slowest for the least bound state.

Sarah Geller transcribed Zwiebach's notes to create the first LaTeX version of this document.

Lecture 12

B. Zwiebach
March 20, 2016

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1 General properties

You will be proving the following facts in your homework:

1. Given the Schrödinger equation with potential $V(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (V(x) - E)\psi = 0 \tag{1.1}$$

there are no energy eigenstates with $E < \min_x V(x)$. In other words, the situation indicated in Fig.1 cannot occur.

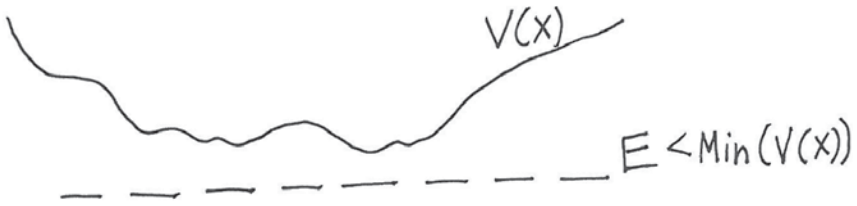

Figure 1: There are no solutions with energy E less than the minimum of the potential $V(x)$.

2. For a one-dimensional potential over $-\infty \le x \le \infty$, there are no degenerate bound states. Recall that a bound state is a normalizable energy eigenstate. Given that, $\lim_{x\to\infty}\psi = 0$.

We now show that the reality of $V(x)$ allows us to work with real wavefunctions $\psi(x)$. Even though there are complex solutions, we can choose real ones without loss of generality.

Theorem 1. The energy eigenstates $\psi(x)$ can be chosen to be real.

Proof. Consider our main equation for the complex wavefunction $\psi(x)$:

$$\psi'' + \frac{2m}{\hbar^2}(E - V(x))\psi \;=\; 0\,. \tag{1.2}$$

Since $(\psi'')^* = (\psi^*)''$ and $V(x)$ is real, the complex conjugation of the above equation gives

$$(\psi^*)'' + \frac{2m}{\hbar^2}(E - V(x))\psi^* \;=\; 0\,. \tag{1.3}$$

We see that $\psi^*(x)$ is another solution of the Schrödinger equation with the *same energy*. The solution $\psi^*(x)$ is different from $\psi(x)$ if there is no constant c such that $\psi^* = c\psi$. In that case ψ^* and ψ represent two degenerate solutions and, by superposition, we can obtain two *real* degenerate solutions:

$$\psi_r \equiv \frac{1}{2}(\psi + \psi^*)\,, \quad \psi_{im} \;\equiv\; \frac{1}{2i}(\psi - \psi^*)\,. \tag{1.4}$$

These are, of course, the real and imaginary parts of ψ. If $\psi^* = c\psi$ the real and imaginary parts yield the same real solution. In either case we can work with a real solution. □

If we are dealing with bound states of one-dimensional potentials more can be said: it is not that we can choose to work with real solutions but rather that any solution is, to begin with, essentially real.

Corollary 1. Any bound state $\psi(x)$ of a one-dimensional potential is real, up to an overall constant phase.

Proof. Recall that in one dimensional potentials there are no degenerate bound states. This means that the two real solutions ψ_r and ψ_{im} considered above must be equal up to a constant that can only be real:

$$\psi_{im}(x) = c\,\psi_r(x)\,, \quad \text{with} \;\; c \in \mathbb{R} \tag{1.5}$$

It then follows that $\psi = \psi_r + i\psi_{im} = (1 + ic)\psi_r$. Writing $1 + ic = \sqrt{1 + c^2}\, e^{i\beta}$ with real β, shows that ψ is, up to a constant phase β, equal to a real solution.

Our next result shows that for a potential that is a symmetric function of x, we can work with energy eigenstates that are either symmetric or antisymmetric functions of x.

Theorem 2. If $V(-x) = V(x)$, the energy eigenstates can be chosen to be even or odd under $x \to -x$.

Proof. Again, we begin with our main equation

$$\psi'' + \frac{2m}{\hbar^2}(E - V(x))\psi \;=\; 0\,. \tag{1.6}$$

Recall that primes denote here derivative with respect to the argument, so $\psi''(x)$ means the function "second-derivative-of-ψ" evaluated at x. Similarly $\psi''(-x)$ means the function "second-derivative-of-ψ" evaluated at $-x$. Thus we can change x for $-x$ with impunity in the above equation getting

$$\psi''(-x) + \frac{2m}{\hbar^2}(E - V(x))\psi(-x) \;=\; 0\,, \tag{1.7}$$

where we used that V is even. We now want to make clear that the above equation implies that $\psi(-x)$ is another solution of the Schrödinger equation with the same energy. For this let us define a function $\varphi(x)$ and take two derivatives of it

$$\varphi(x) \;\equiv \psi(-x) \quad \to \quad \frac{d}{dx}\varphi(x) \;=\; \psi'(-x)\cdot(-1)\,, \qquad \frac{d^2}{dx^2}\,\varphi(x) \;=\; \psi''(-x)\,. \tag{1.8}$$

Using the last equation (1.7) becomes

$$\frac{d^2}{dx^2}\,\varphi(x) + \frac{2m}{\hbar^2}(E - V(x))\varphi(x) \;=\; 0\,. \tag{1.9}$$

showing that $\varphi(x) = \psi(-x)$ provides a degenerate solution to the Schrödinger equation: Equipped with the degenerate solutions $\psi(x)$ and $\psi(-x)$ we can now form symmetric (s) and antisymmetric (a) combinations that are, respectively, even and odd under $x \to -x$:

$$\psi_s(x) \equiv \frac{1}{2}(\psi(x) + \psi(-x)), \quad \psi_a(x) \equiv \frac{1}{2}(\psi(x) - \psi(-x)). \tag{1.10}$$

These are the solutions claimed to exist. □
Note that the above proof would not work for the case of odd potentials $V(-x) = -V(x)$. We can't say much in this case!

Again, if we focus on *bound states* of one-dimensional even potentials the absence of degeneracy has a stronger implication: the solutions are automatically even or odd.

Corollary 2. Any bound state of a one-dimensional even potential is either even or odd.

Proof: The absence of degeneracy implies that the solutions $\psi(x)$ and $\psi(-x)$ must be the same solution. Because of corollary 1, we can choose $\psi(x)$ to be real and thus we must have

$$\psi(-x) = c\,\psi(x), \quad \text{with } c \in \mathbb{R}. \tag{1.11}$$

Letting $x \to -x$ in the above equation we get $\psi(x) = c\psi(-x) = c^2\psi(x)$ from which we learn that $c^2 = 1$. The only possibilities are $c = \pm 1$. So $\psi(x)$ is *automatically* even or odd under $x \to -x$. □

We used the result of this theorem to find the bound states of the finite square well. Since that potential is even, we could restrict our work to search for even bound states and odd bound states. The potential cannot have bound states that are neither even nor odd!

2 Bound states in slowly varying potentials

We will now consider some insights that classical physics gives us about the behavior of energy eigenstates. This is sometimes called the **semi-classical approximation** because classical physics can sometime give an approximate description of the quantum physics.

We begin with an example we already understand. We consider the total energy E of a particle that is the sum of a potential energy V and a kinetic energy K. When V is a function of position, K must also be a function of position in order for the sum E to be conserved, as it must be. In our first example, shown in Figure 2, the potential V is constant and the energy E is greater than V. A particle in such a potential will have a constant potential energy K and thus a constant momentum $p = \sqrt{2mK}$. It is a fact that the wave representing the quantum particle has a de Broglie wavelength λ equal to Planck's constant h divided by the classical momentum.

Indeed from the Schrödinger equation

$$\psi'' = -\frac{2m}{\hbar^2}(E - V)\psi = -\frac{2mK}{\hbar^2}\psi = -\frac{p^2}{\hbar^2}\psi, \tag{2.1}$$

leading to real solutions of the form

$$\psi \sim \cos\Big(\frac{p}{\hbar}x\Big) = \cos\Big[\frac{2\pi}{(h/p)}x\Big], \tag{2.2}$$

where we see that the wavelength of ψ is the de Broglie wavelength of a particle with momentum p. This wavefunction is real and thus is not a momentum eigenstate. It represents a superposition of a

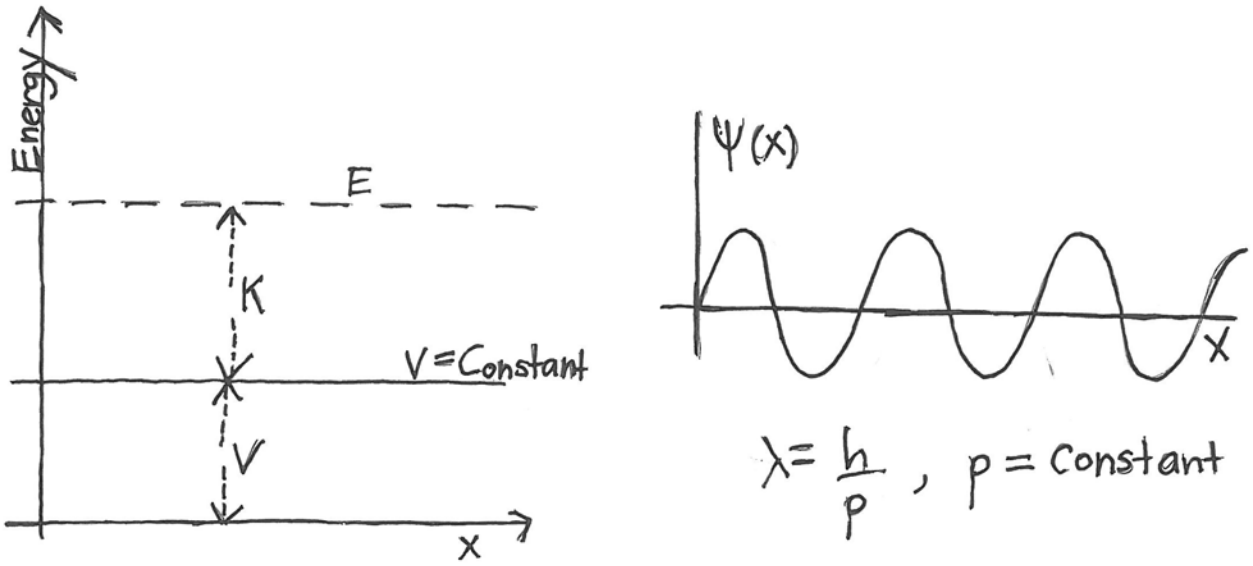

Figure 2: On the left is an example of a constant potential, $V = V_0 < E$ where K is kinetic energy, and $E = K + V_0$ is the total energy. On the right is a sketch of the wavefunction for a particle in this potential. Constant $V \implies$ constant K, thus momentum is also constant.

.

state with momentum p and a state of momentum $-p$. Even in the classical case, the kinetic energy K only determines p^2 and not the sign of p. Our interest here is in real wavefunctions $\psi(x)$ as appropriate for *energy eigenstates* and what we have seen is that, for a constant potential, the wavelength of $\psi(x)$ is the de Broglie wavelength associated to the classical momentum.

Consider now the situation depicted in figure 3, where we imagine a classical particle moving in a linearly increasing potential $V(x)$. This time the kinetic energy $K(x)$ is also position dependent. As a result, the momentum of the classical particle $p(x) = \sqrt{2mK(x)}$ is also position dependent. The insight now is that, if the potential is slowly varying, to a good approximation the wavefunction will have a position-dependent de Broglie wavelength $\lambda(x)$ given by

$$\lambda(x) \;=\; \frac{h}{p(x)}\,. \tag{2.3}$$

By this we mean that ψ is some combination of functions

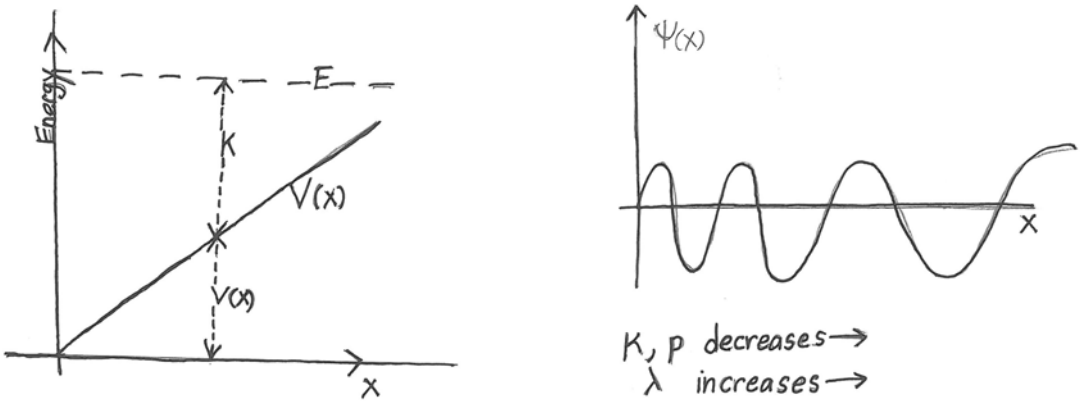

Figure 3: A linearly varying potential, $V(x) = \alpha x$. The energy $E = K + V(x)$ is fixed, and as x increases $K(x)$ decreases, $p(x)$ decreases, and $\lambda(x)$ increases, resulting in a wavefunction of increasing wavelength.

$$\cos\Big(\frac{2\pi x}{\lambda(x)}\Big)\,, \quad \sin\Big(\frac{2\pi x}{\lambda(x)}\Big)\,. \tag{2.4}$$

As we see in Figure 3, because of the linearly growing $V(x)$ a particle with total energy E will have decreasing kinetic energy $K(x)$ as x increases. Thus the classical momentum will decrease, and we anticipate that the wavefunction will have an increasing local de Broglie wavelength $\lambda(x)$ as x increases. This is illustrated to the right of the figure. We will discuss below what we expect to happen to the amplitude of the wavefunction.

The semiclassical approximation – setting the $\psi(x)$ wavelength equal to the de Broglie wavelength of the classical particle – is accurate when the potential changes slowly. By slowly we mean that the change in the potential over a distance comparable to the local de-Broglie wavelength is very small compared to the potential:

$$\lambda(x)\left|\frac{dV}{dx}\right| \ll |V(x)|\,. \tag{2.5}$$

The left side of the inequality is an estimate for the change in V over a distance $\lambda(x)$, and therefore this quantity must be very small compared to the potential for the semiclassical approximation to be valid. This inequality above is the key condition for the semiclassical approximation. It is in fact the condition that allows one to set up the WKB analysis of the Schrödinger equation (8.06!).

In figure 4 we show an arbitrary potential $V(x)$ and consider the classical motion of a particle of total energy E. For any point x_0, we have $V(x_0) + K(x_0) = E$. The maximum kinetic energy occurs for the minimum value of the potential. Classically a particle cannot have negative kinetic energy, thus the particle cannot be found at points where $V(x)$ is greater than the energy E. In the figure, this happens for $x > x_R$ and for $x < x_L$, and these regions are called classically forbidden regions. A particle of energy E will oscillate from x_L to x_R and back. As it moves its velocity changes, it is a function $v(x)$ of position. The points x_L and x_R are called **turning points**, because at these points the particle motion reverses direction.

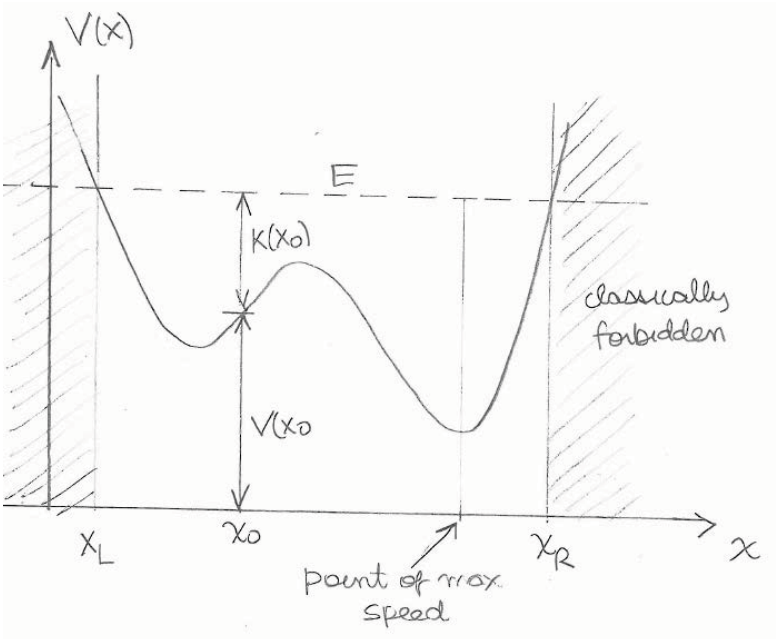

Figure 4: An arbitrary potential showing turning points x_L and x_R. The region to the right of x_R and the region to the left of x_L are classically forbidden regions. At any point $x \in [x_L, x_R]$ the sum of the potential energy $V(x)$ and the kinetic energy $K(x)$ is equal to the total energy E.

The oscillating classical particle spends more time in the regions where its velocity is small and less time in the regions where its velocity is large. This has quantum mechanical implications. Indeed, in the semiclassical approximation we find that the wavefunction amplitude is bigger at the places the particle spends more time and smaller at places it spends less time. This can be quantified. Consider the probability $|\psi(x)|^2 dx$ to find the particle within the infinitesimal region dx around x. This is set this proportional to the fraction of time the particle spends at dx:

$$|\psi(x)|^2 dx \simeq \frac{dt}{T} . \tag{2.6}$$

where dt the time require to traverse dx and T is the half-period of oscillation, the time to go from the left turning point to the right turning point. With $v(x)$ the local velocity of the particle, we have

$$|\psi(x)|^2 dx \simeq \frac{dx}{v(x)T} = \frac{m}{T}\frac{1}{p(x)}dx \quad \rightarrow \quad |\psi(x)|^2 \sim \frac{1}{p(x)} . \tag{2.7}$$

This relation has to be interpreted with some care. Recall that $\psi(x)$ has very small wavelength for large $p(x)$. So $|\psi(x)|^2$ oscillates between zero and some peak value over very short distances along x. On the other hand, the momentum $p(x)$ appearing on the right has no such oscillations. Therefore, by $|\psi(x)|^2$ in the above relation we really mean the average of $|\psi(x)|^2$ over a few oscillations near x, in other words the square of the **amplitude** of the wave $\psi(x)$. Writing the amplitude (a positive real number, of course) as $\mathrm{Amp}(\psi(x))$, we have

$$\boxed{\mathrm{Amp}(\psi(x)) \sim \frac{1}{\sqrt{p(x)}} \sim \sqrt{\lambda(x)} .} \tag{2.8}$$

The amplitude of the wave is proportional to the square root of the de Broglie wavelength. Thus in figure 5, the momentum of the particle decreases and $\lambda(x)$ increases as x increases. So we expect the amplitude of the wave to increase, as sketched to the right.

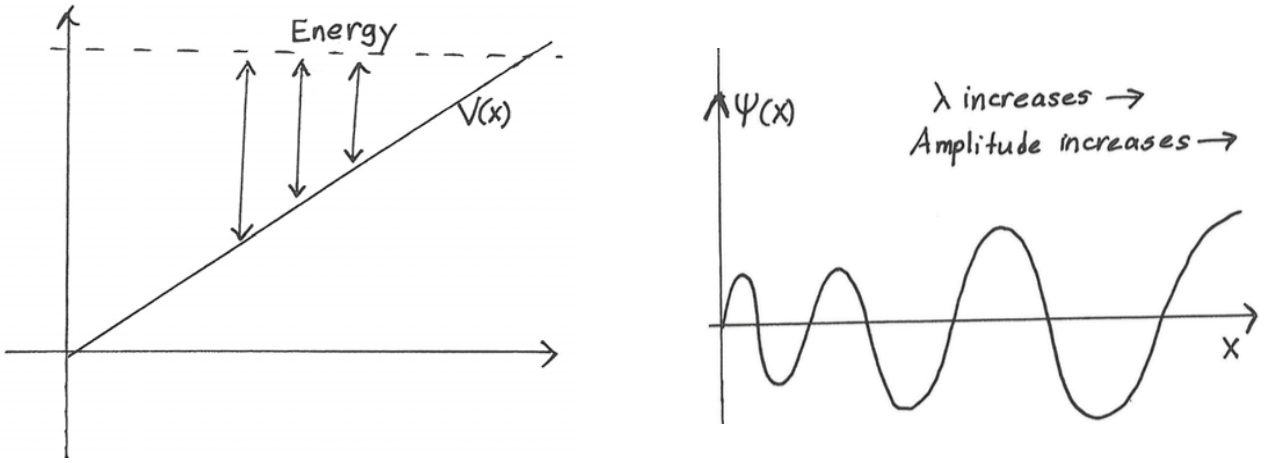

Figure 5: A potential $V(x)$ and a kinetic energy that decreases for increasing x. Then the de Broglie wavelength increases with x. Equation 2.8 then implies that the amplitude of $\psi(x)$ also increases with x.

As a simple illustration of the importance of averaging $|\psi|^2$ consider a state of large energy in the infinite well potential, as shown in Fig. 6. Within the box, the classical particle "bounces" between the walls with constant velocity. As a result the particle spends the same amount of time in every equal

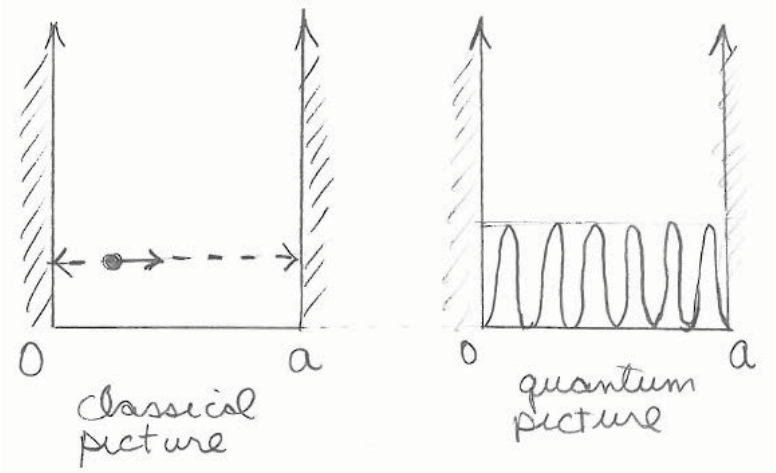

Figure 6: Particle in a one dimensional box. The particle bounces with constant velocity.

size interval dx within the box. The classical probability distribution $\mathbb{P}_{\rm cl}$ within the box is uniform:

$$\mathbb{P}_{\rm cl}(x)dx \;=\; \frac{1}{a}\,dx \quad \to \quad \mathbb{P}_{\rm cl}(x) \;=\; \frac{1}{a}\,, \tag{2.9}$$

since the integral over the box $x \in [0,a]$ of $\mathbb{P}_{\rm cl}(x)dx$ gives one. Now consider an energy eigenstate $\psi_n(x)$ with large n

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \quad \to \quad |\psi_n(x)|^2 = \frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right). \tag{2.10}$$

The associated quantum-mechanical probability density $\mathbb{P}_{\rm qm}$ is

$$\mathbb{P}_{\rm qm}(x) = |\psi_n(x)|^2 = \frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right), \tag{2.11}$$

and it is, for large n a rapidly oscillating function, seemingly quite different from the classical probability $\mathbb{P}_{\rm cl} = 1/a$. While the classical probability never vanishes, the quantum probability has many zeroes! Still, over arbitrary distances larger than the a/n (presumed small since n is very large) the average of the quantum probability density is approaches the classical probability density. Recall that the average of $\sin^2$ over any integer number of oscillations is $1/2$, so that its average over *any* interval that includes a large number of oscillations (not necessarily integer) is approximately equal to $1/2$. We then have

$$\text{Average}_x(\mathbb{P}_{\rm qm}(x)) \simeq \;\frac{2}{a}\cdot\frac{1}{2} \;=\; \frac{1}{a} = \mathbb{P}_{\rm cl}(x)\,. \tag{2.12}$$

The semiclassical approximation is an explicit realization of what is loosely called the "Correspondence principle", the idea that there are limits of quantum states in which their properties can be understood by a classical analysis of the system.

3 Sketching wavefunction behavior in different regions

Let's examine the behavior of an energy eigenstate for the case of a general potential $V(x)$. We rewrite the time-independent Schrödinger equation by dividing by ψ to get:

$$\frac{\psi''(x)}{\psi(x)} = -\frac{2m}{\hbar^2}(E - V(x)), \tag{3.1}$$

which is convenient because there is no wavefunction on the right-hand side. We will consider the equation in two regions and at some special points.

- $E - V(x) < 0$, classically forbidden region because the total energy is smaller than the potential. In this case the right hand side of eqn. (3.1) is positive. This means there are two possibilities: both ψ and ψ'' are positive or both ψ and ψ'' are negative. These possibilities are shown here

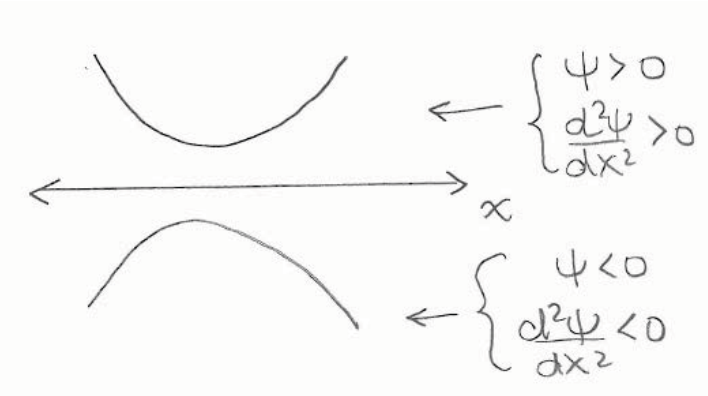

Figure 7: In the classically forbidden region either $\psi > 0$, $\psi'' > 0$ or $\psi < 0$, $\psi'' < 0$. In both cases the wavefunction is *convex towards* the x-axis.

Such possible behaviors are summarized by saying that **the wavefunction is convex towards the axis.** When classically forbidden regions reach to $x = -\infty$ or $x = \infty$ the behavior is of the type shown below:

Figure 8: Wavefunctions approaching $x = -\infty$ or $x = \infty$ within classically forbidden regions.

- $E - V > 0$, classically allowed region: the right hand side of eqn. 3.1 is negative. Thus either $\psi > 0, \psi'' < 0$ or one has $\psi < 0, \psi'' > 0$. Both options are shown below and are summarized by saying that **the wavefunction is concave towards the axis:**

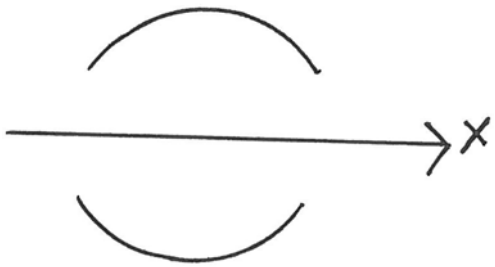

Figure 9: $\psi > 0$, $\psi'' < 0$ or $\psi < 0$, $\psi'' > 0$. The wavefunction is *concave towards* the x-axis.

A classically allowed region that is large would have the the top and bottom parts of the figure above alternating to form a function resembling a sin or cos.

- $V(x_0) = E$. Turning point: defined as a point x_0 at which the potential energy $V(x_0)$ is equal to the total energy E. Turning points separate classically allowed and classically forbidden regions. A turning point is an **inflection point** in the graph of $\psi(x)$, a point where the second derivative vanishes, since

$$\psi''\big|_{x_0} = -\frac{2m}{\hbar^2} \cdot 0 \cdot \psi(x_0) = 0, \tag{3.2}$$

Not all inflection points are turning points. In fact nodes of the wavefunction are inflection points. This is clear from $\psi'' = -\frac{2m}{\hbar^2}(E - V(x))\psi$, since vanishing ψ implies vanishing ψ''.

Note, however, that having vanishing ψ and ψ' at any point in the domain of the wavefunction is not allowed. This is because the Schrödinger equation is a second order linear differential equation. One can quickly show that $\psi = \psi'$ at some point x_0 implies that all higher derivatives of ψ vanish at that point. Assuming the wavefunction has a Taylor expansion we conclude that the wavefunction must vanish identically.

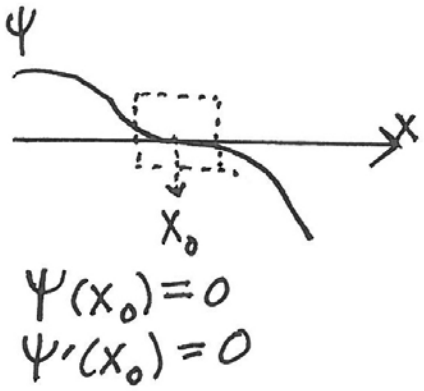

Figure 10: It is impossible to have both ψ and ψ' at any point x_0: the Schrödinger equation would then force $\psi(x)$ to vanish identically.

We conclude this section by illustrating the quantization of the energy levels for bound states of an even potential. As shown in Figure 11, at the top, we have an even potential and we have marked four energies $E_1 < E_2 < E_3 < E_4$. Not all correspond to energy eigenstates. We imagine integrating the Schrödinger equation from $x = \infty$ down to $x = 0$. As shown in the small figure slightly to the right and below the potential, we assume $\psi > 0$ as $x \to \infty$. Since any bound state is automatically even or odd, the picture at $x \to -\infty$ must either the one with $\psi > 0$ (the even extension) or the one

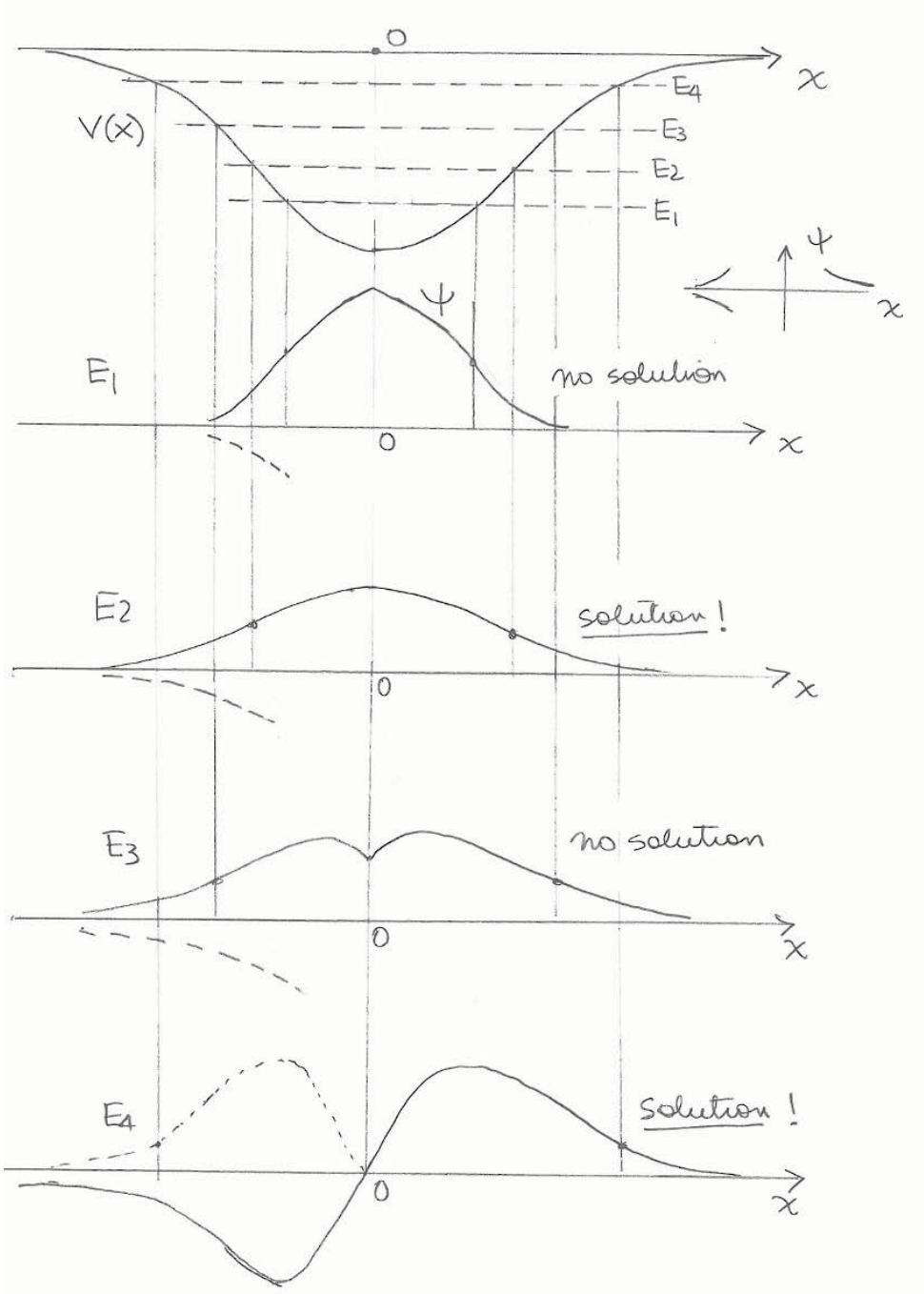

Figure 11: An even potential (top figure) and the result of integrating the equation from $x = \infty$ towards zero for various values of the energy. We get a solution when $\psi(x)$ for $x \geq 0$ can be matched with continuous ψ and ψ' to an even or odd extension valid for $x < 0$. There is no solution for E_1 and E_3. The ground state arises for E_2 and the first excited state arises for E_4.

with $\psi < 0$ (the odd extension). To have a solution, the picture from the right must match properly at $x = 0$ with one of the two possible extensions at $x < 0$.

Consider, for example, the integration of the equation for $E = E_1$. Coming in from $x = \infty$ the solution has an inflection point and becomes concave towards the axis. Beyond this point the first derivative ψ' decreases. Still, as shown in the picture ψ' does not vanish at $x = 0$, so that the even extension for $x < 0$ does not match properly with the $x > 0$ solution at $x = 0$, because ψ' fails to be continuous. Matching with the odd extension is not a possibility because then ψ would fail to be continuous at $x = 0$. Thus E_1 is not an allowed energy.

As we increase the energy to $E = E_2$, the turning point occurs for larger x and ψ' manages to get exactly to zero at $x = 0$, matching ψ and ψ' from the even extension. This time we have a solution. Of course this occurs for $E = E_2$ precisely; a bit more energy or a bit less energy and the derivative is not continuous at $x = 0$.

As we increase the energy to E_3 the turning point moves to even larger x and ψ' is negative by the time we get to $x = 0$, while ψ is still positive. The solution can't be matched with the even extension because of the discontinuous derivative.

If we now increase the energy further to some value E_4, by the time we reach $x = 0$ the derivative ψ' will be negative and ψ will be exactly zero. As you can see in the figure, we can get a good match to the odd extension for $x < 0$. This is the first excited state. It is an odd wavefunction with a single node at $x = 0$.

4 Shooting Method

The **shooting method** is a numerical method to find the form of bound-state solution to the the Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi = 0\,. \tag{4.1}$$

The method is easily implemented for even potentials $V(x)$ in which case we can search for even and for odd bound states.

Consider first even bound states. We will attempt to integrate the differential equation from $x = 0$ to $x = \infty$. To start at $x = 0$ we need to fix ψ and ψ' at this point. Since the normalization of the bound state is not determined by the equation, we can choose

$$\psi(x = 0) \;=\; 1\,. \tag{4.2}$$

The derivative must also be zero at this point: if the derivative is not zero the even wavefunction will have a discontinuous derivative at $x = 0$ (can you see that?). Therefore we must set

$$\psi'(x = 0) \;=\; 0\,. \tag{4.3}$$

To integrate the differential equation we now need to choose some energy. Pick some arbitrary value E_0. We know already that arbitrary values of the energy do not yield bound states. So what goes wrong if we now integrate the differential equation. What happens typically is that you get a solution that could not be normalized. As you work with your computer you notice that beyond certain point along x the solution diverges, perhaps by having $\psi \to \infty$, that is ψ going up.

You must then change the value of the energy until you find some value E_1 for which the solution also diverges, but this time with $\psi \to -\infty$, or ψ going down. This is a signal that there is some energy in the interval between E_0 and E_1 for which a normalizable solution exists. You then try to narrow the interval. If $E_0 < E_1$ you can do that by finding values larger than E_0 for which the divergence is still up and values lower than E_1 for which the divergence is still down. As you narrow the interval

you will still find these divergences, but they occur for larger and larger values of x. As you do so, you are getting a better and better approximation to the bound-state energy (see Fig.12).

For odd solutions, the procedure is the same, but the boundary conditions at $x = 0$ are:

$$\begin{aligned} \psi(x=0) &= 0\,, \\ \psi'(x=0) &= 1\,. \end{aligned} \tag{4.4}$$

The first is needed for a continuous odd function. The second is arbitrary, up to normalization.

If a potential is not even but has a hard wall, this provides a good starting point for integration of the Schrödinger equation. At this point the wavefunction is set to zero and the derivative set to one. If the potential has two hard walls, we can integrate starting from one wall and then demand that the solution reach exactly zero by the time we get to the second wall.

A practical note: When working with computers to carry out these numerical integrations, it is first necessary to "clean out" the units from the differential equation. The first step in this process is to replace x for a unit free variable u. The relation between them is of the form $x = bu$ where b is a quantity with units of length built from the parameters in the problem.

Figure 12: Numerical integration of the Schrödinger equation leads to solutions that diverge up ($\psi \to \infty$) or down ($\psi \to -\infty$) beyond some value of x. Bound states are found for values of energies at which the divergence changes from up to down, or from down to up.

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 13: Delta Function Potential, Node Theorem, and Simple Harmonic Oscillator

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April 1, 2016

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1 The Delta Function Potential

Consider a particle of mass m moving in a one-dimensional potential. The potential $V(x)$ is is rather singular: it vanishes for all x except for $x = 0$ at which point it has infinite strength. More precisely, the potential is delta function localized at $x = 0$ and is written as

$$V(x) = -\alpha\,\delta(x), \quad \alpha > 0\,, \tag{1.1}$$

Here α is a constant chosen to be positive. Because of the explicit minus sign, the potential is infinitely negative at $x = 0$; the potential is attractive. The potential is shown in Fig. 1, where we represent the delta function by an arrow pointing downwards.

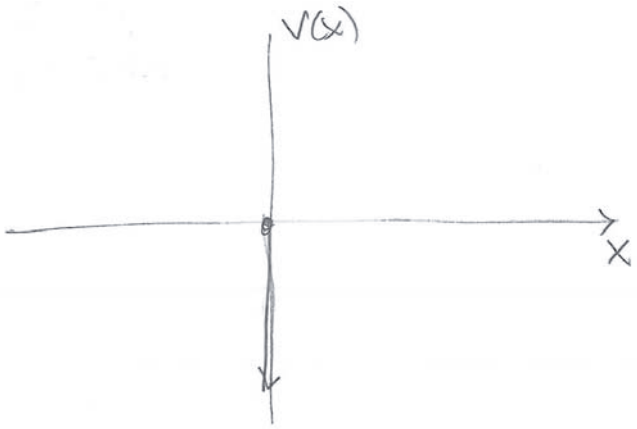

Figure 1: A delta function well.

We want to know if this potential admits bound states. For a bound state the energy E must be negative: this ensures that all of $x \neq 0$ is classically forbidden, and the wavefunction will decay rapidly allowing a normalized solution. A bit of intuition comes by thinking of the delta function as approximated by a finite square well in the limit as the width of the well goes to zero and the depth goes to infinity in such a way that the product, representing the "area" is finite (the delta function is a function with unit area, as it is clear from its integral). In Figure 2 we show two finite-well representations and sketch the wavefunction. We can see that the middle region provides the curving

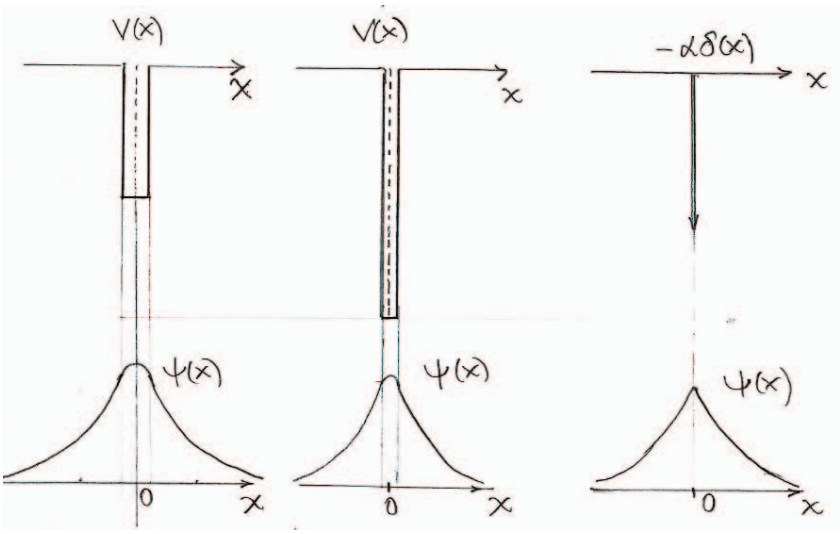

Figure 2: The delta function potential viewed as the limit as the finite square well becomes narrower and deeper simultaneously. We expect to get a wavefunction with discontinuous derivative.

of the wavefunction needed to have a smooth derivative. In the limit as the width of the region goes to zero we would expect, if there is a bound state, to have *discontinuous* derivative.

We can get further insight by considering units. The dimension-full constants in the problem are α, m, and $\hbar$. Since a delta function has units of one over length, the constant α must have units of energy times length for the potential to have units of energy. Thus we have, as units

$$E \;=\; \frac{\alpha}{L}\,, \tag{1.2}$$

but, as usual, the units of energy are

$$E \;=\; \frac{\hbar^2}{mL^2}\,. \tag{1.3}$$

From these two equations we find

$$L \;=\; \frac{\hbar^2}{m\alpha} \quad\rightarrow\quad E \;=\; \frac{m\alpha^2}{\hbar^2}\,. \tag{1.4}$$

The units of energy must be carried by the above combination of the constants of the problem. Therefore the energy E_b of any bound state must be a number times that combination:

$$E_b \;=\; -\,\#\,\frac{m\alpha^2}{\hbar^2}\,. \tag{1.5}$$

where # is a unit free positive number that we aim to determine. It is good to see α appearing in the numerator. This means that as the strength of the delta function increases, the depth of the bound state also increases, as we would naturally expect!

Let us now turn to the relevant equations. We want to find an $E < 0$ state. The wavefunction is constrained by the time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E - V(x))\psi. \tag{1.6}$$

For $x \neq 0$, we have $V(x) = 0$, so this becomes

$$\frac{d^2\psi}{dx^2} = \left(-\frac{2mE}{\hbar^2}\right)\psi = \kappa^2\psi, \qquad \kappa^2 \equiv -\frac{2mE}{\hbar^2} > 0. \tag{1.7}$$

The solutions to this differential equation are of the form

$$e^{\kappa x}, \quad e^{-\kappa x}, \quad \kappa > 0\,. \tag{1.8}$$

The potential is even: $\delta(-x) = \delta(x)$, so if we have a ground state it must be even and, of course, have no nodes. If there is an excited state, it must be odd and thus have a node at $x = 0$. The only odd solution we can build with the above exponentials is $\sinh \kappa x$. But a $\psi \sim \sinh \kappa x$ cannot be normalized, it blows up at $x = \pm\infty$. Therefore there cannot be an excited state in the delta function potential. If there are bound states there is just one of them!

Let us use the above solutions to build the the ground state wavefunction. First, we can see that for $x > 0$ we must discard the solution $e^{\kappa x}$, because it diverges as $x \to \infty$. Similarly we must discard $e^{-\kappa x}$ for $x < 0$. Since the wavefunction must be continuous at $x = 0$ the solution must be of the form

$$\psi(x) = \begin{cases} A\, e^{-\kappa x} & x > 0\,, \\ A\, e^{\kappa x} & x < 0\,. \end{cases} \tag{1.9}$$

Is any value of κ allowed for this solution? No, we will get another constraint by considering the derivative of the wavefunction and learning that, as anticipated, it is discontinuous. Indeed, the Schrödinger equation gives us a constraint for this discontinuity. Starting with

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi\,, \tag{1.10}$$

we integrate this equation from $-\epsilon$ to ϵ, with $0 < \epsilon \ll 1$, a range that includes the position of the delta function. This gives

$$-\frac{\hbar^2}{2m}\left(\left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}\right) + \int_{-\epsilon}^{\epsilon} dx\ (-\alpha\delta(x))\psi(x) = E\int_{-\epsilon}^{\epsilon} dx\ \psi(x)\,. \tag{1.11}$$

The integral on the left-hand side returns a finite value due to the delta function. In the limit as $\epsilon \to 0$ the integral on the right-hand side vanishes because $\psi(x)$ is finite for all x, while the region of integration is contracting away. This yields

$$-\frac{\hbar^2}{2m}\lim_{\epsilon\to 0}\left(\left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}\right) - \alpha\psi(0) = 0\,. \tag{1.12}$$

We define the discontinuity Δ_0 of ψ' at $x = 0$ as

$$\Delta_0\left(\frac{d\psi}{dx}\right) \equiv \lim_{\epsilon\to 0}\left(\left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}\right). \tag{1.13}$$

We have therefore learned that

$$\boxed{\Delta_0\left(\frac{d\psi}{dx}\right) = -\frac{2m\alpha}{\hbar^2}\,\psi(0)\,.} \tag{1.14}$$

Note that the discontinuity in ψ' at the position of the delta function is proportional to the value of the wavefunction at that point. At a node a delta function would have no effect; ψ' would also be continuous.

Applying the discontinuity equation to our solution (1.9), we have

$$\lim_{\epsilon\to 0}\Big(\left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}\Big) = \lim_{\epsilon\to 0}\Big(-\kappa A e^{-\kappa\epsilon} - \kappa A e^{-\kappa\epsilon}\Big) = -2\kappa A \;=\; -\frac{2m\alpha}{\hbar^2}A\,. \tag{1.15}$$

This relation fixes the value of κ

$$\kappa \;=\; \frac{m\alpha}{\hbar^2}\,, \tag{1.16}$$

and therefore the value E_b of the bound state energy

$$E_b = -\frac{\hbar^2\kappa^2}{2m} = -\frac{1}{2}\cdot\frac{m\alpha^2}{\hbar^2}. \tag{1.17}$$

As we anticipated with the unit analysis, the answer takes the required form (1.5) and the undetermined constant # takes the value 1/2.

2 The Node Theorem

Recall the infinite well potential

$$V(x) = \begin{cases} 0 & 0 < x < a\,, \\ \infty & \text{elsewhere.} \end{cases} \tag{2.18}$$

The bound states take the form

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\Big(\frac{n\pi x}{a}\Big) \tag{2.19}$$

and corresponding energies

$$E_n = \frac{\hbar^2 n^2}{2ma^2}\,, \quad n = 1, 2, \ldots \tag{2.20}$$

Note that ψ_n has $n-1$ nodes (zeroes). (The points $x = 0$ and $x = a$ are *not* nodes, but rather endpoints.)

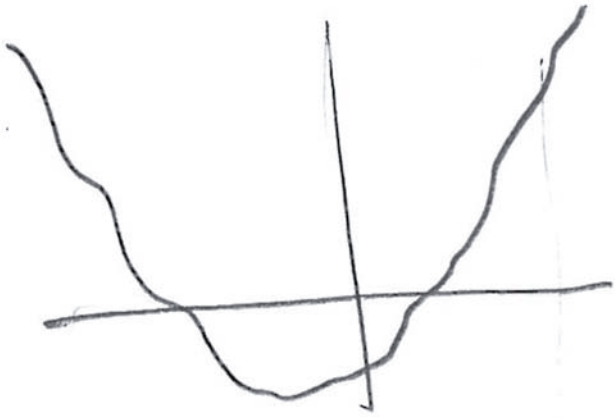

Figure 3: A smooth potential that goes to infinity as $|x| \to \infty$.

This leads us to the *node theorem*. Consider a potential $V(x)$ that is continuous and satisfies $V(x) \to \infty$ as $|x| \to \infty$ (Fig. 3). This potential has a number of bound states (energy eigenstates that satisfy $\psi \to 0$ as $|x| \to \infty$), which we index $\psi_1, \psi_2, \psi_3, \ldots$. Recall also that there are no degenerate bound states in one dimension. The node theorem states that ψ_n has $n-1$ nodes. We will give an intuitive, non-rigorous explanation of this phenomenon.

For this argument we also recall that $\psi(x_0) = \psi'(x_0) = 0$ implies that $\psi(x) = 0$ for all x. One cannot have vanishing derivative at a zero of the wavefunction. That applies to nodes or finite endpoints.

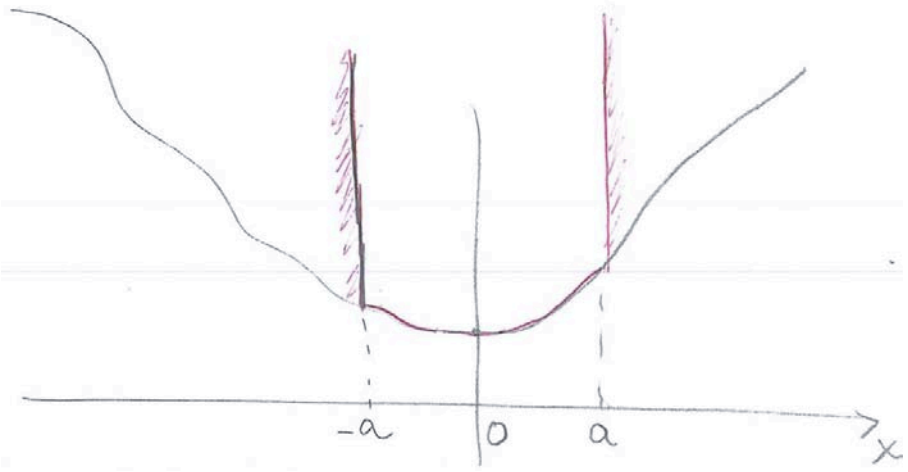

Figure 4: The screened potential $V_a(x)$.

First, we examine the potential and fix the location of $x = 0$ at a minimum. We then define the *screened* potentials $V_a(x)$ as follows:

$$V_a(x) = \begin{cases} V(x) & |x| < a\,, \\ \infty & |x| > a\,. \end{cases} \tag{2.21}$$

As shown in Fig. 4, the screened potential $V_a(x)$ is an infinite well of width $2a$ whose bottom is the taken from $V(x)$. The argument below is based on two plausible assumptions. First: As $a \to \infty$ the bound states of $V_a(x)$ become the bound states of $V(x)$. Second: As a is increased the wavefunction and its derivative are continuously stretched and deformed.

When a is very small, $V_a(x)$ is approximately a very narrow infinite well with a flat bottom – an infinite *square* well. This is because we chose $x = 0$ to be a minimum and any minimum is locally flat. On this infinite square well the node theorem holds. The ground state, for example, will vanish at the endpoints and will have no nodes. We will now argue that as the screen is enlarged we can't generate a node. This applies to the ground state, as we explicitly discuss below, and to all other states too. If we can't generate nodes by screen enlargement the node theorem applies to $V(x)$.

Why is this the case? Consider how we might develop an additional node while stretching the screen. To start with, consider the ground state in the top part of Figure 5. There is no node at this value of the screen and we have $\psi'(-a) > 0$ (left wall) and $\psi'(a) < 0$ (right wall). Suppose that as we increase a we produce a node, shown for the larger screen a' below. For this to happen the sign of ψ' at one of the endpoints must change. In the case shown it is the right endpoint that experiences a change in the sign of ψ'. With the assumption of continuous stretching there would have to be some intermediate screen at which $\psi' = 0$ at the right endpoint. But in that case, $\psi = \psi' = 0$ at this endpoint, and then $\psi(x) = 0$ for all x, which is clearly impossible.

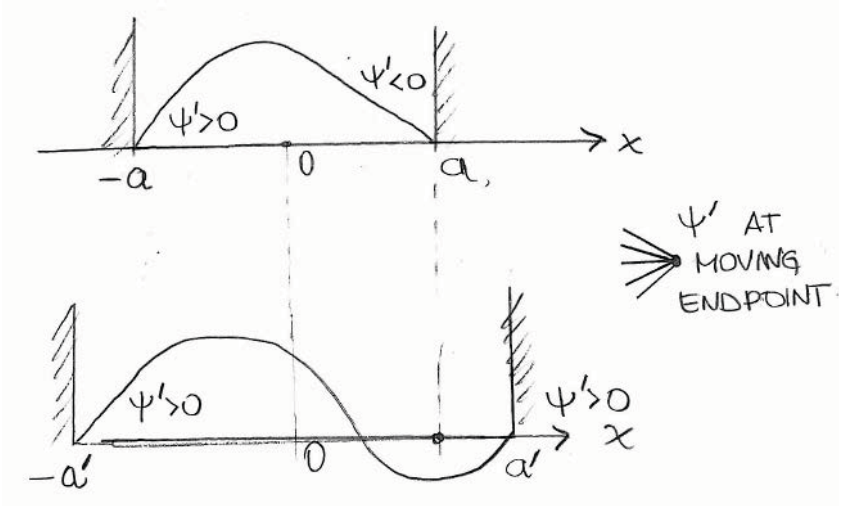

Figure 5: Introducing a single node requires changing the sign of the derivative at the right endpoint: $\psi'(a) < 0$ but $\psi'(a') > 0$. At some intermediate screen, the value of ψ' at the right endpoint must become zero. But this is impossible.

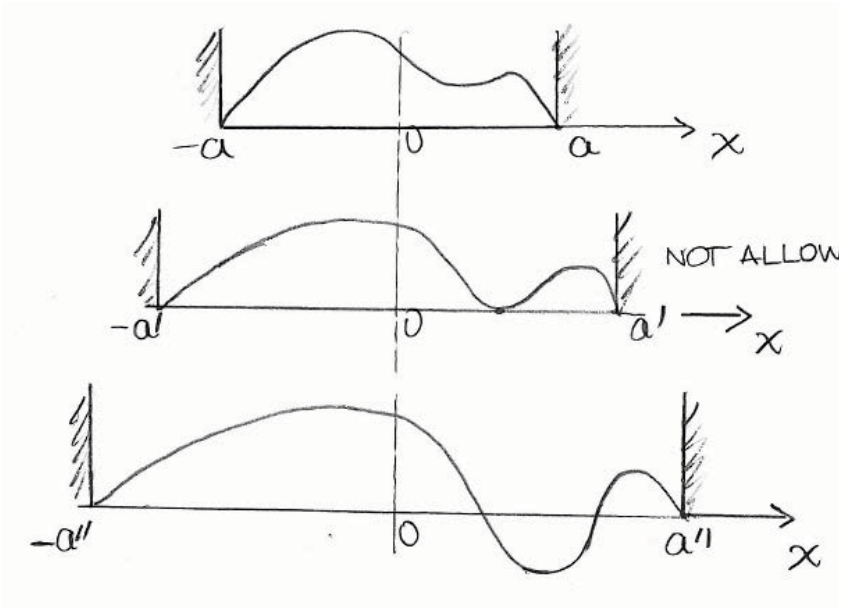

Figure 6: Introducing two nodes by having the wavefunction cross the x-axis in between the two boundaries (compare top and bottom). This is not possible as it would require in an intermediate screen (middle) in which $\psi = \psi' = 0$ at some point.

It is possible to introduce nodes without changing the sign of ψ' at either endpoint. In this process, shown in Fig. 6, the wavefunction dips and produces two new nodes. This process can't take place, however. Indeed, for some intermediate screen the wavefunction must be tangential to the x axis and at this point we will have $\psi = \psi' = 0$, which is impossible.

We conclude that we cannot change the number of nodes of *any* wavefunction as we stretch the screen. The n-th excited state of the tiny infinite square well, with $n-1$ nodes will turn into the n-th excited state of $V(x)$ with $n-1$ nodes. In the tiny infinite square well the energy levels are ordered

in increasing energy by the number of nodes. The same is true at all stages of the stretching screen and therefore for true for $V(x)$. Any two consecutive energy levels cannot get permuted because, by continuity, this would require a situation where we have a degeneracy, which is not possible.

3 Harmonic Oscillator

The classical harmonic oscillator is a rich and interesting dynamical system. It allows us to understand many kinds of oscillations in complex systems. The total energy E of a particle of mass m moving in one dimension under the action of a restoring force $F = -kx$, $k > 0$, is usually written as

$$E \;=\; \tfrac{1}{2}\, mv^2 + \tfrac{1}{2} kx^2 \,. \tag{3.22}$$

The first term is the kinetic energy and the second term is the potential energy

$$V(x) = \tfrac{1}{2} kx^2 \,. \tag{3.23}$$

The potential is quadratic in x. In such a system the particle performs oscillatory motion with angular frequency ω given by

$$\omega \;=\; \sqrt{\frac{k}{m}} \quad \to \quad k \;=\; m\omega^2 \,. \tag{3.24}$$

Trading k for ω and using the momentum to express the kinetic energy, we can rewrite E as follows

$$E \;=\; \frac{p^2}{2m} \;+\; \tfrac{1}{2} m\omega^2\, x^2 \,. \tag{3.25}$$

This is all for the classical harmonic oscillator.

The quadratic potential is ubiquitous in physics, as it arises to first approximation when we expand an *arbitrary* potential around a minimum. To show this consider an arbitrary potential $V(x)$ with a minimum at x_0. For $x \approx x_0$, we can use a Taylor expansion to write

$$V(x) \;=\; V(x_0) + (x - x_0)V'(x_0) + \tfrac{1}{2}(x - x_0)^2 V''(x_0) + \mathcal{O}((x - x_0)^3) \,. \tag{3.26}$$

Since x_0 is a critical point $V'(x_0) = 0$. Dropping the higher order terms, we then have that the potential is approximately quadratic

$$V(x) \approx V(x_0) + \tfrac{1}{2} V''(x_0)(x - x_0)^2. \tag{3.27}$$

This is a good approximation for x close to x_0. Since x_0 is a minimum $V''(x_0) > 0$ and this is a harmonic oscillator centered at x_0 and with $k = V''(x_0)$. The additive constant $V(x_0)$ has no effect on the dynamics.

Faced with the question of defining a *quantum* harmonic oscillator we are inspired by the above expression (3.25) for the energy and *declare* that $\hat{x}$ and $\hat{p}$ will be operators with $[\hat{x}, \hat{p}] = i\hbar$ and that the Hamiltonian $\hat{H}$ is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \tfrac{1}{2} m\omega^2 \hat{x}^2, \qquad [\,\hat{x},\, \hat{p}\,] = i\hbar \,. \tag{3.28}$$

The harmonic oscillator potential in here is

$$V(x) = \tfrac{1}{2}\, m\omega^2 x^2. \tag{3.29}$$

Note that ω has units of frequency: $[\omega] = 1/T$. We can use this to construct a characteristic energy $\hbar\omega$. The quantum harmonic oscillator is a rather natural system directly inspired by the classical oscillator.

Our first step is finding the energy eigenstates, the solutions of the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\varphi(x) = E\varphi(x). \tag{3.30}$$

Here both E and $\varphi(x)$ are unknown. We expect that energy eigenstates only exist for certain quantized values of E.

As a first step we will clean the equation of dimensionful constants. This helps us appreciate better the equation at hand. Moreover, it would allow us to easily put the equation on a computer. Each term in the equation must have units of energy times units of φ, as we can see by looking at the right-hand side of the equation. Note that the units of φ are not relevant to the consistency of the equation, as φ appears on each term. We can therefore ignore the units of φ. The units of energy on the left- hand side are constructed on the first term by a combination of constants and derivatives and in the second term by a combination of constants and powers of x. If we could work with a unit free coordinate u instead of x the units of energy would have to be produced *just* by the constants in the problem, and as we have seen, the only possibility is $\hbar\omega$. A common $\hbar\omega$ factor will then simplify tremendously the structure of the equation as it will allow us to define a unit free energy!

We therefore begin by introducing a unit-free coordinate u to replace the conventional coordinate x. We set

$$x \;=\; a\,u, \qquad u \text{ unit free}, \quad [a] = L\,, \tag{3.31}$$

where a must be a constant with units of length. To determine a in terms of $\hbar, m$, and ω we equate a characteristic kinetic energy to a characteristic potential energy:

$$\frac{\hbar^2}{ma^2} \;=\; m\omega^2 a^2 \quad \to \quad a^2 \;=\; \frac{\hbar}{m\omega}\,. \tag{3.32}$$

Now, plugging $x = au$ into the time-independent Schrödinger equation yields

$$-\frac{\hbar^2}{2ma^2}\frac{d^2\varphi(u)}{du^2} + \frac{1}{2}m\omega^2 a^2 u^2\varphi(u) = E\varphi(u). \tag{3.33}$$

Here, we have used

$$\frac{d}{dx} = \frac{du}{dx}\frac{d}{du} = \frac{1}{a}\frac{d}{du}. \tag{3.34}$$

Note that $\frac{\hbar^2}{ma^2} = \hbar\omega$ and $m\omega^2 a^2 = \hbar\omega$, so we have

$$-\tfrac{1}{2}\hbar\omega\frac{d^2\varphi(u)}{du^2} + \tfrac{1}{2}\hbar\omega u^2\varphi(u) = E\varphi(u). \tag{3.35}$$

We can see that things are working. As expected the energy units on the left-hand side are carried by $\hbar\omega$! Multiplying by $\frac{2}{\hbar\omega}$, we reach

$$-\frac{d^2\varphi(u)}{du^2} + u^2\varphi(u) \;=\; \mathcal{E}\varphi(u), \tag{3.36}$$

where we have defined a unit free energy $\mathcal{E}$:

$$\mathcal{E} \;\equiv\; \frac{2E}{\hbar\omega}\,, \quad E \;=\; \tfrac{1}{2}\hbar\omega\,\mathcal{E}\,. \tag{3.37}$$

If we know the pure number $\mathcal{E}$ we then know the energy E. Rearranging, we reach the cleaned-up version of the time-independent Schrödinger equation:

$$\boxed{\frac{d^2\varphi}{du^2} \;=\; (u^2-\mathcal{E})\varphi\;.} \tag{3.38}$$

This is our simplified, unit free version of the time-independent Schrödinger equation. It is clearly less cluttered than (3.30).

The above differential equation must have solutions for all values of the energy parameter $\mathcal{E}$, after all you could integrate it on a computer! Quantization must arise because solutions are not normalizable except for special values of $\mathcal{E}$. To understand this issue as it relates to the equation we examine solutions for large values of $|u|$. In this limit, $\mathcal{E}$ can be ignored as compared to u^2, and we have the approximate equation

$$\varphi''(u) \;\approx\; u^2\varphi(u). \tag{3.39}$$

This equation cannot be solved by any polynomial! If φ is a polynomial of degree n, the degree of the left hand side would be $n-2$ and that of the right-hand side $n+2$. This cannot work. Let's try a solution of the form

$$\varphi(u) \;=\; u^k e^{\alpha u^2/2}. \tag{3.40}$$

The leading term in φ'' comes when we differentiate the exponential:

$$\varphi''(u) \;\approx\; \alpha^2 u^2\varphi(u) \quad \text{as } |u|\to\infty. \tag{3.41}$$

Comparing with (3.39) we have solutions for $\alpha=\pm 1$, in which case we have

$$\varphi(u) \;\approx\; Au^k e^{-u^2/2} + Bu^k e^{u^2/2} \quad \text{as } |u|\to\infty\,. \tag{3.42}$$

The solution with coefficient B would not yield an energy eigenstate because it diverges as $|u|\to\infty$ and would not be normalizable. Note that the u^k factor played no role in the analysis. This factor, however suggests that a polynomial multiplying $e^{\pm u^2/2}$ could be a solution of the differential equation.

This analysis suggests that, for our purposes, we should write

$$\varphi(u) = h(u)e^{-u^2/2}\,. \tag{3.43}$$

Note that there is no assumption or loss of generality in writing this expression. Indeed, any function $\varphi(u)$ and be written some other function times $e^{-u^2/2}$ as it is immediately clear $(\varphi(u)e^{u^2/2})e^{-u^2/2}$. In writing (3.43) we are only hoping that the differential equation for $h(u)$ is simpler. Clearly, if we find $h(u)$ we have found $\varphi(u)$. We actually expect that $h(u)$ may be a polynomial because the ansatz captures the large $|u|$ dependence that prevents the solution for $\varphi(u)$ from being a polynomial.

Plugging (3.43) into (3.38) and simplifying, we find a second-order linear differential equation for $h(u)$:

$$\boxed{\frac{d^2h}{du^2} - 2u\frac{dh}{du} + (\mathcal{E}-1)h = 0\,.} \tag{3.44}$$

It is actually possible at this point to see that getting a polynomial solution requires quantization of $\mathcal{E}$ Indeed, assume that $h(u)$ is a polynomial of degree j:

$$h(u) \;=\; u^j + \alpha_1 u^{j-1} + \alpha_2 u^{j-2} + \ldots\,. \tag{3.45}$$

In the above equation the first term is then a polynomial of degree $j-2$. Each of the other two terms are polynomials of degree j. For the equation to make sense the coefficient of contributions to the coefficient of u^j and u^{j-1} must vanish. The coefficient of u^j is

$$\text{Coefficient of } \; u^j : \quad -2j + \mathcal{E} - 1 = 0 \quad \rightarrow \quad \mathcal{E} = 2j + 1 \, . \tag{3.46}$$

Thus, we get the quantization of energy: a polynomial solution $h(u)$ of degree j requires $\mathcal{E} = 2j + 1$. You may wonder about the subleading term of degree $j-1$ whose coefficient must also vanish.

$$\text{Coefficient of } \; u^{j-1} : \quad (-2(j-1) + \mathcal{E} - 1)\alpha_1 = 0 \, . \tag{3.47}$$

Since the energy $\mathcal{E}$ has already been fixed, the only way to satisfy this condition is to set $\alpha_1 = 0$. Thus the polynomial is actually of the form

$$h(u) \; = \; u^j + \alpha_2 u^{j-2} + \ldots \, . \tag{3.48}$$

If this is supposed to lead to an energy eigenstate the vanishing of α_1 could have been anticipated. Since the harmonic oscillator potential is even we know that bound states *must be* either even or odd. Since $e^{-u^2/2}$ is even, the solution $\varphi(u)$ will be either even or odd if $h(u)$ is even or odd. If α_1 had not vanished, $h(u)$ would have two consecutive powers of u and could not be either even or odd.

We can analyze the equation more systematically using a series expansion:

$$h(u) = \sum_{k=0}^{\infty} a_k u^k . \tag{3.49}$$

A simple way to plug into the differential equation (3.44) is to select from each term the contribution to the coefficient of u^j. For this one can imagine the terms $a_j u^j + a_{j+1} u^{j+1} + a_{j+2} u^{j+2}$ in $h(u)$ and select the piece that contributes to the coefficient of u^j:

$$\begin{aligned} \text{Contribution from: } \; \frac{d^2 h}{du^2} \; &: \quad (j+2)(j+1) a_{j+2} \\ \text{Contribution from: } \; -2u \frac{dh}{du} \; &: \quad -2j a_j \\ \text{Contribution from: } \; (\mathcal{E}-1)h \; &: \quad (\mathcal{E}-1) a_j \end{aligned} \tag{3.50}$$

The total coefficient of u^j in the left hand side of the differential equation must be set to zero, for all values of j, for the differential equation to be satisfied. Therefore

$$(j+2)(j+1)a_{j+2} - 2j a_j + (\mathcal{E}-1) a_j \; = \; 0 \, , \qquad j = 0, 1, 2, \ldots \tag{3.51}$$

This can be written as a recursion relation:

$$a_{j+2} = \frac{2j + 1 - \mathcal{E}}{(j+2)(j+1)} \, a_j \, , \tag{3.52}$$

This is a two-step recurrence relation. If you choose some a_0 you can construct a solution that contains only odd coefficients, $a_2, a_4, \ldots$ as determined recursively by the above relation. That solution, of the form

$$a_0 + a_2 u^2 + a_4 u^4 + \cdots \tag{3.53}$$

would be even. Another solution is constructed by choosing some a_1 and then using the above recursion to find $a_3, a_5, \ldots$. That solution, of the form

$$a_1 u + a_3 u^3 + \cdots . \tag{3.54}$$

would be odd. For any arbitrary value of $\mathcal{E}$ both solutions of the differential equation (3.44) exist, but neither one would be polynomial and neither one would be expected to be a good energy eigenstate. The general solution to (3.44) with arbitrary $\mathcal{E}$ is thus determined by the two constants (a_0, a_1) as they together determine all coefficients. This makes sense, because $a_0 = h(0)$ and $a_1 = h'(0)$ and the solution of a second order differential equation is be determined by knowing the function and its derivative at any point.

Let us now demonstrate that if the series for $h(u)$ never stops the corresponding $\varphi(u)$ is not an acceptable energy eigenstates. Let us see what would be the large u behavior of $h(u)$ if it does not terminate. For large j the recursion relation (3.52) gives

$$\frac{a_{j+2}}{a_j} \approx \frac{2}{j} . \tag{3.55}$$

What kind of function grows this way? Note that

$$e^{u^2} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(u^2\right)^n = \sum_{j\in \text{ even}} \frac{1}{(j/2)!} u^j . \tag{3.56}$$

This series has coefficients $c_j = \frac{1}{(j/2)!}$ for even j, and so we see that

$$\frac{c_{j+2}}{c_j} = \frac{(j/2)!}{((j+2)/2)!} = \frac{2}{j+2} \approx \frac{2}{j} , \tag{3.57}$$

for large j. This is just the behavior noted in (3.55) for $h(u)$. So, if the series for $h(u)$ does not terminate the wavefunction is behaves like

$$\varphi(u) = h(u) e^{-u^2/2} \sim e^{u^2} e^{-u^2/2} \sim e^{u^2/2}, \tag{3.58}$$

which is the bad solution we identified in (3.42). This proves that $h(u)$ must be a polynomial and the recursion relation must terminate for us to get an energy eigenstate!

Now we discuss how to get a polynomial $h(u)$, although the main conclusion was anticipated earlier in (3.46). If $h(u)$ is to be of degree j it must have non vanishing a_j and *vanishing* a_{j+2}, as determined from the recursion relation (3.52). The numerator in this recursion relation must vanish and we must choose $\mathcal{E}$ such that

$$2j + 1 - \mathcal{E} = 0 . \tag{3.59}$$

The solution will then take the form:

$$h(u) = a_j u^j + a_{j-2} u^{j-2} + \cdots , \tag{3.60}$$

with powers decreasing in steps of two because this is what the recursion relation demands for having a solution. The solution will therefore be automatically even (if j is even) or odd (if j is odd). Say j is even and the solution is even with energy $2j + 1$ as required. The second solution of the differential equation for that value of the energy would be odd, but the energy $2j + 1$ that made the even solution

terminate will not make the odd solution terminate. This means that the second solution of the differential equation is not an energy eigenstate.

We usually call the degree j of the solution using the letter n. Then,

$$\mathcal{E} = 2n + 1\,, \quad n = 0, 1, 2, \ldots \tag{3.61}$$

corresponds to the polynomial solution

$$h_n(u) \;=\; a_n u^n \;+ a_{n-2} u^{n-2} + \cdots\;, \quad n = 0, 1, 2, \ldots \tag{3.62}$$

The energy of the solution $\varphi_n(u) = h_n(u) e^{-u^2/2}$ is

$$E = \frac{\hbar\omega}{2}\mathcal{E} = \frac{\hbar\omega}{2}(2n+1). \tag{3.63}$$

We have

$$E_n = \hbar\omega\Big(n + \frac{1}{2}\Big)\,, \quad n = 0, 1, 2, \ldots \tag{3.64}$$

We see that the energies are quantized and the energy levels are evenly spaced. The ground state energy is $E_0 = \hbar\omega/2$. The corresponding power series solutions $h_n(u)$ are the Hermite polynomials, usually denoted as $H_n(u)$

$$H_n(u) = 2^n u^n \pm \cdots\,. \tag{3.65}$$

The factor of 2^n here is a convention choice. The Hermite polynomials are solutions of (3.44) with $\mathcal{E} = 2n + 1$ therefore they satisfy the differential equation

$$\frac{d^2 H_n}{du^2} - 2u\frac{dH_n}{du} + 2nH_n = 0. \tag{3.66}$$

The first several Hermite polynomials are

$$\begin{aligned} H_0(u) &= 1 \\ H_1(u) &= 2u \\ H_2(u) &= 4u^2 - 2 \\ H_3(u) &= 8u^3 - 12u\,. \end{aligned} \tag{3.67}$$

The generating function for the Hermite polynomials is an exponential, with formal parameter z:

$$e^{-z^2+2zu} = \sum_{u=0}^{\infty} \frac{z^n}{n!} H_n(u). \tag{3.68}$$

It is not too hard to show that the polynomials defined by this expansion satisfy the requisite differential equation (3.66) and are normalized as claimed in (3.65).

Let us write the energy eigenstates in terms of x. Recalling that $u^2 = x^2/a^2$, where $a^2 = \frac{\hbar}{m\omega}$ the relation

$$\varphi_n(u) \;\sim\; H_n(u) e^{-u^2/2}, \tag{3.69}$$

then gives us

$$\varphi_n(x) \;=\; N_n\, H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) e^{-\frac{m\omega}{2\hbar}x^2} \quad n = 0, 1, 2, \ldots\,, \tag{3.70}$$

where N_n is a normalization constant.

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 14 and 15: Algebraic approach to the SHO

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1 Algebraic Solution of the Oscillator

We have already seen how to calculate energy eigenstates for the simple harmonic oscillator by solving a second-order differential equation, the time-independent Schrödinger equation.

Let us now try to factorize the harmonic oscillator Hamiltonian. By this we mean, roughly, writing the Hamiltonian as the product of an operator times its *Hermitian conjugate*. As a first step we rewrite the Hamiltonian as

$$\hat{H} \;=\; \tfrac{1}{2}m\omega^2\Big(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\Big)\,. \tag{1.1}$$

Motivated by the identity $a^2+b^2 = (a-ib)(a+ib)$, holding for numbers a and b, we examine if the expression in parenthesis can be written as a product

$$\begin{aligned}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) \;&=\; \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} + \frac{i}{m\omega}\big(\hat{x}\hat{p} - \hat{p}\hat{x}\big)\,,\\ &=\; \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} - \frac{\hbar}{m\omega}\mathbf{1}\,,\end{aligned} \tag{1.2}$$

where the extra terms arise because $\hat{x}$ and $\hat{p}$, as opposed to numbers, do not commute. We now define the right-most factor in the above product to be V:

$$V \;\equiv\; \hat{x} + \frac{i\hat{p}}{m\omega}\,, \tag{1.3}$$

Since $\hat{x}$ and $\hat{p}$ are Hermitian operators, we then have

$$V^\dagger \;=\; \hat{x} - \frac{i\hat{p}}{m\omega}\,, \tag{1.4}$$

and this is the left-most factor in the product! We can therefore rewrite (1.2) as

$$\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} \;=\; V^\dagger V + \frac{\hbar}{m\omega}\mathbf{1}\,, \tag{1.5}$$

and therefore back in the Hamiltonian (1.1) we find,

$$\hat{H} \;=\; \tfrac{1}{2}m\omega^2\, V^\dagger V \;+\; \tfrac{1}{2}\hbar\omega\mathbf{1}\,. \tag{1.6}$$

This is a factorized form of the Hamiltonian: up to an additive constant E_0, $\hat{H}$ is the product of a positive constant times the operator product $V^\dagger V$. We note that the commutator of V and $V^\dagger$ is simple

$$\big[V\,,V^\dagger\big] \;=\; \Big[\hat{x}+\frac{i\hat{p}}{m\omega}\,,\hat{x}-\frac{i\hat{p}}{m\omega}\Big] \;=\; -\frac{i}{m\omega}[\hat{x}\,,\hat{p}]+\frac{i}{m\omega}[\hat{p},\hat{x}] \;=\; \frac{2\hbar}{m\omega}\mathbf{1}\,. \tag{1.7}$$

This implies that

$$\left[\sqrt{\frac{m\omega}{2\hbar}}\,V\;,\;\sqrt{\frac{m\omega}{2\hbar}}\,V^\dagger\right] =\; 1\;. \tag{1.8}$$

This suggests the definition of unit-free operator operators $\hat{a}$ and $\hat{a}^\dagger$:

$$\begin{aligned}\hat{a} \;&\equiv\; \sqrt{\frac{m\omega}{2\hbar}}\,V\,,\\ \hat{a}^\dagger \;&\equiv\; \sqrt{\frac{m\omega}{2\hbar}}\,V^\dagger\,.\end{aligned} \tag{1.9}$$

Due to the scaling we have

$$\boxed{\big[\,\hat{a}\,,\hat{a}^\dagger\,\big]=\mathbf{1}\,.} \tag{1.10}$$

The operator $\hat{a}$ is called *annihilation* operator and $\hat{a}^\dagger$ is called a *creation* operator. The justification for these names will be seen below. From the above definitions we read the relations between $(\hat{a},\hat{a}^\dagger)$ and $(\hat{x}\,,\hat{p})$:

$$\boxed{\begin{aligned}\hat{a} \;&=\; \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}+\frac{i\hat{p}}{m\omega}\right)\;,\\ \hat{a}^\dagger \;&=\; \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}-\frac{i\hat{p}}{m\omega}\right)\;.\end{aligned}} \tag{1.11}$$

The inverse relations are many times useful as well,

$$\boxed{\begin{aligned}\hat{x} \;&=\; \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger)\;,\\ \hat{p} \;&=\; i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger-\hat{a})\,.\end{aligned}} \tag{1.12}$$

While neither $\hat{a}$ nor $\hat{a}^\dagger$ is hermitian (they are hermitian conjugates of each other), the above equations are consistent with the hermiticity of $\hat{x}$ and $\hat{p}$. We can now write the Hamiltonian in terms of the $\hat{a}$ and $\hat{a}^\dagger$ operators. Using (1.9) we have

$$V^\dagger V \;=\; \frac{2\hbar}{m\omega}\,\hat{a}^\dagger\hat{a}\,, \tag{1.13}$$

and therefore back in (1.6) we get

$$\boxed{\hat{H} \;=\; \hbar\omega\big(\hat{a}^\dagger\hat{a}+\tfrac{1}{2}\big) \;=\; \hbar\omega\big(\hat{N}+\tfrac{1}{2}\big)\,,\quad \hat{N}\;\equiv\;\hat{a}^\dagger\hat{a}\,.} \tag{1.14}$$

The above form of the Hamiltonian is factorized: up to an additive constant $\hat{H}$ is the product of a positive constant times the operator product $\hat{a}^\dagger\hat{a}$. In here we have dropped the identity operator, which

is usually understood. We have also introduced the *number* operator $\hat{N}$. This is, by construction, a hermitian operator and it is, up to a scale and an additive constant, equal to the Hamiltonian. An eigenstate of $\hat{H}$ is also an eigenstate of $\hat{N}$ and it follows from the above relation that the respective eigenvalues E and N are related by

$$E \;=\; \hbar\omega\left(N+\tfrac{1}{2}\right). \tag{1.15}$$

Let us now show the powerful conclusions that arise from the factorized Hamiltonian. On any state ψ that is normalized we have

$$\langle\hat{H}\rangle_\psi \;=\; \big(\psi,\hat{H}\psi\big) \;=\hbar\omega\big(\psi,\hat{a}^\dagger\hat{a}\psi\big)+\tfrac{1}{2}\hbar\omega\big(\psi,\psi\big)\,, \tag{1.16}$$

and moving the $\hat{a}^\dagger$ to the first input, we get

$$\langle\hat{H}\rangle_\psi \;=\; \hbar\omega\big(\hat{a}\psi\,,\hat{a}\psi\big)+\tfrac{1}{2}\hbar\omega \;\geq\; \tfrac{1}{2}\hbar\omega\,. \tag{1.17}$$

The inequality follows because any expression of the form (φ,φ) is greater than or equal to zero. This shows that for any energy eigenstate with energy E: $\hat{H}\psi=E\psi$ we have

$$\text{Energy eigenstates:}\;\; E \;\geq\; \tfrac{1}{2}\hbar\omega\,. \tag{1.18}$$

This important result about the spectrum followed directly from the factorization of the Hamiltonian. But we also get the information required to find the ground state wavefunction. The minimum energy $\frac{1}{2}\hbar\omega$ will be realized for a state ψ if the term $\big(\hat{a}\psi\,,\hat{a}\psi\big)$ in (1.17) vanishes. For this to vanish $\hat{a}\psi$ must vanish. Therefore, the ground state wavefunction φ_0 must satisfy

$$\hat{a}\,\varphi_0=0\,. \tag{1.19}$$

The operator $\hat{a}$ annihilates the ground state and this why $\hat{a}$ is called the annihilation operator. Using the definition of $\hat{a}$ in (1.11) and the position space representation of $\hat{p}$, this becomes

$$\left(x+\frac{i}{m\omega}\frac{\hbar}{i}\frac{d}{dx}\right)\varphi_0(x)=0 \quad\to\quad \left(x+\frac{\hbar}{m\omega}\frac{d}{dx}\right)\varphi_0(x)=0\,. \tag{1.20}$$

Remarkably, this is a **first order** differential equation for the ground state. Not a second order equation, like the Schrödinger equation that determines the general energy eigenstates. This is a dramatic simplification afforded by the factorization of the Hamiltonian into a product of first-order differential operators. The above equation is rearranged as

$$\frac{d\varphi_0}{dx}=-\frac{m\omega}{\hbar}\,x\varphi_0\,. \tag{1.21}$$

Solving this differential equation yields

$$\boxed{\;\varphi_0(x) \;=\; \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}\,,\;} \tag{1.22}$$

where we included a normalization constant to guarantee that $(\varphi_0,\varphi_0)=1$. Note that φ_0 is indeed an energy eigenstate with energy E_0:

$$\hat{H}\varphi_0 \;=\hbar\omega\big(\hat{a}^\dagger\hat{a}+\tfrac{1}{2}\big)\varphi_0 \;=\tfrac{1}{2}\hbar\omega\varphi_0 \quad\to\quad E_0 \;=\; \tfrac{1}{2}\,\hbar\omega\,. \tag{1.23}$$

Before proceeding with the analysis of excited states, let us view the properties of factorization more generally. Factorizing a Hamiltonian means finding an operator $\hat{A}$ such that we can rewrite the Hamiltonian as $\hat{A}^\dagger A$ up to an additive constant. Here $\hat{A}^\dagger$ is the Hermitian conjugate of $\hat{A}$, an operator that is defined by

$$\big(\psi, \hat{A}^\dagger \varphi\big) \;=\; \big(\hat{A}\psi\,, \varphi\big)\,. \tag{1.24}$$

We say that we have factorized a Hamiltonian $\hat{H}$ if we can find a $\hat{A}$ for which

$$\boxed{\hat{H} \;=\; \hat{A}^\dagger \hat{A} \;+\; E_0\,\mathbf{1}\,,} \tag{1.25}$$

where E_0 is a constant with units of energy that multiplies the identity operator. This constant does not complicate our task of finding the eigenstates of the Hamiltonian, nor their energies: any eigenfunction of $\hat{A}^\dagger\hat{A}$ is an eigenfunction of $\hat{H}$. Two key properties follow from the factorization (1.25).

1. Any energy eigenstate must have energy greater than or equal to E_0. First note that for an *arbitrary* normalized $\psi(x)$ we have

   $$\big(\psi\,, \hat{H}\psi\big) \;=\; \big(\psi\,, \hat{A}^\dagger\hat{A}\,\psi\big) + E_0\big(\psi\,,\psi\big) \;=\big(\hat{A}\psi\,, \hat{A}\psi\big) + E_0\,, \tag{1.26}$$

   Since the overlap $(\hat{A}\psi, \hat{A}\psi)$ is greater than or equal to zero, we have shown that

   $$\boxed{\big(\psi\,, \hat{H}\psi\big) \;\geq\; E_0\,.} \tag{1.27}$$

   If we take ψ to be an energy eigenstate of energy E: $\hat{H}\psi = E\psi$, the above relation gives

   $$E \geq E_0\,. \tag{1.28}$$

   This shows, as claimed, that all possible energies are greater than or equal to E_0.

2. A wavefunction ψ_0 that satisfies

   $$\hat{A}\,\psi_0 \;=\; 0\,, \tag{1.29}$$

   is an energy eigenstate that *saturates* the inequality (1.28). Indeed,

   $$\hat{H}\psi_0 \;=\; \hat{A}^\dagger\hat{A}\,\psi_0 + E_0\psi_0 \;=\; \hat{A}^\dagger(\hat{A}\,\psi_0) + E_0\psi_0 \;=\; E_0\psi_0\,. \tag{1.30}$$

   The state ψ_0 satisfying $\hat{A}\,\psi_0 = 0$ is the ground state. For conventional Hamiltonians this is a first order differential equation for ψ_0 and much easier to solve than the Schrödinger equation.

2 Operator manipulation and the spectrum

We have seen that all energy eigenstates are eigenstates of the Hermitian number operator $\hat{N} = \hat{a}^\dagger\hat{a}$. This is because $\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$. Note that since $\hat{a}\varphi_0 = 0$ we also have

$$\hat{N}\varphi_0 = 0\,. \tag{2.1}$$

We can quickly check that

$$\begin{aligned} \big[\hat{N},\hat{a}\big] \;&=\; \big[\hat{a}^\dagger\hat{a},\hat{a}\big] \;=\; \big[\hat{a}^\dagger,\hat{a}\big]\,\hat{a} \;=\; -\hat{a}\,, \\ \big[\hat{N},\hat{a}^\dagger\big] \;&=\; \big[\hat{a}^\dagger\hat{a},\hat{a}^\dagger\big] \;=\; \hat{a}^\dagger\big[\hat{a},\hat{a}^\dagger\big] \;=\; \hat{a}^\dagger\,, \end{aligned} \tag{2.2}$$

which we summarize as

$$\begin{aligned} \big[\,\hat{N},\,\hat{a}\,\big] \;&=\; -\,\hat{a}\,, \\ \big[\,\hat{N},\,\hat{a}^\dagger\,\big] \;&=\; \hat{a}^\dagger\,. \end{aligned} \tag{2.3}$$

Using these identities and induction you should be able to show that:

$$\begin{aligned} \big[\,\hat{N},(\hat{a})^k\,\big] \;&=\; -k\,(\hat{a})^k\,, \\ \big[\,\hat{N},\;(\hat{a}^\dagger)^k\,\big] \;&=\; k\,(\hat{a}^\dagger)^k. \end{aligned} \tag{2.4}$$

These relations suggest why $\hat{N}$ is called the number operator. Acting on powers of creation or annihilation operators by commutation it gives the same object multiplied by (plus or minus) the number of creation or annihilation operators, k in the above. Closely related commutators are also useful:

$$\begin{aligned} \big[\,\hat{a}^\dagger\,,(\hat{a})^k\,\big] \;&=\; -k\,(\hat{a})^{k-1} \\ \big[\,\hat{a}\,,\;(\hat{a}^\dagger)^k\,\big] \;&=\; k\,(\hat{a}^\dagger)^{k-1}. \end{aligned} \tag{2.5}$$

These commutators are analogous to $[\hat{p},(\hat{x})^k]$ and $[\hat{x},(\hat{p})^k]$. We will also make use of the following Lemma which helps in evaluations where we have an operator $\hat{A}$ that kills a state ψ and we aim to simplify the action of $\hat{A}\hat{B}$, where $\hat{B}$ is another operator, acting on ψ. Here is the result

$$\boxed{\text{If } \hat{A}\,\psi = 0\,,\ \text{then}\ \ \hat{A}\,\hat{B}\,\psi \;=\; \big[\,\hat{A}\,,\,\hat{B}\,\big]\psi\,.} \tag{2.6}$$

This is easily proved. First note that

$$\hat{A}\hat{B} \;=\; [\hat{A},\hat{B}] + \hat{B}\hat{A}\,, \tag{2.7}$$

as can be quickly checked expanding the right-hand side. It then follows that

$$\hat{A}\,\hat{B}\,\psi \;=\; \big([\hat{A},\hat{B}] + \hat{B}\hat{A}\big)\psi \;=\; \big[\,\hat{A}\,,\,\hat{B}\,\big]\psi\,, \tag{2.8}$$

because $\hat{B}\hat{A}\,\psi = \hat{B}(\hat{A}\psi) = 0$. This is what we wanted to show. This is all we need to know about commutators and we can now proceed to construct the states of the harmonic oscillator.

Since $\hat{a}$ annihilates φ_0 consider acting on the ground state with $\hat{a}^\dagger$. It is clear that $\hat{a}^\dagger$ cannot also annihilate φ_0. If that would happen acting with both sides of the commutator identity $[\hat{a}\,,\hat{a}^\dagger] = 1$ on φ_0 would lead to a contradiction: the left-hand side would vanish but the right-hand side would not. Thus consider the wavefunction

$$\varphi_1 \;\equiv\; \hat{a}^\dagger\varphi_0\,. \tag{2.9}$$

We are going to show that this is an energy eigenstate. For this purpose we act on it with the number operator:

$$\hat{N}\varphi_1 = \hat{N}\hat{a}^\dagger\varphi_0 \;=\; [\hat{N},\hat{a}^\dagger]\varphi_0\,, \tag{2.10}$$

where we noted that $\hat{N}\varphi_0 = 0$ and used Lemma (2.6). Given that $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$, we get

$$\hat{N}\varphi_1 \ = \hat{a}^\dagger\varphi_0 = \varphi_1. \tag{2.11}$$

Thus φ_1 is an eigenstate of the operator $\hat{N}$ with eigenvalue $N = 1$. Since φ_0 has $\hat{N}$ eigenvalue zero, the effect of acting on φ_0 with $\hat{a}^\dagger$ was to increase the eigenvalue of the number operator by one unit. The operator $\hat{a}^\dagger$ is called the *creation* operator because it creates a state out of the ground state. Alternatively, it is called the *raising* operator, because it raises (by one unit) the eigenvalue of $\hat{N}$. Since $N = 1$ for φ_1 it follows that φ_1 is an energy eigenstate with energy E_1 given by

$$E_1 = \hbar\omega(1 + \tfrac{1}{2}) \ = \ \tfrac{3}{2}\hbar\omega. \tag{2.12}$$

It also turns out that φ_1 is properly normalized:

$$(\varphi_1, \varphi_1) = (\hat{a}^\dagger\varphi_0, \hat{a}^\dagger\varphi_0) = (\varphi_0, \hat{a}\hat{a}^\dagger\varphi_0)\,, \tag{2.13}$$

where we used the Hermitian conjugation property to move the $\hat{a}^\dagger$ acting on the left input into the right input, where it goes as $(\hat{a}^\dagger)^\dagger = \hat{a}$. We then have

$$(\varphi_1, \varphi_1) = (\varphi_0, \hat{a}\hat{a}^\dagger\varphi_0) = (\varphi_0, [\hat{a}, \hat{a}^\dagger]\varphi_0) = (\varphi_0, \varphi_0) = 1, \tag{2.14}$$

where we used (2.6) in the evaluation of $\hat{a}\hat{a}^\dagger\psi_0$. Indeed the state φ_1 is correctly normalized.

Next consider the state

$$\varphi_2' \ \equiv \ \hat{a}^\dagger\hat{a}^\dagger\varphi_0. \tag{2.15}$$

This has

$$\hat{N}\varphi_2' \ = \hat{N}\hat{a}^\dagger\hat{a}^\dagger\varphi_0 \ = \ \left[\hat{N}, \hat{a}^\dagger\hat{a}^\dagger\right]\varphi_0 = 2\hat{a}^\dagger\hat{a}^\dagger\varphi_0 = 2\varphi_2'\,, \tag{2.16}$$

so φ_2 is a state with number $N = 2$ and energy $E_2 = \frac{5}{2}\hbar\omega$. Is it properly normalized? We find

$$\begin{aligned}\big(\varphi_2, \varphi_2\big) = \big(\hat{a}^\dagger\hat{a}^\dagger\varphi_0, \hat{a}^\dagger\hat{a}^\dagger\varphi_0\big) \ &= \big(\varphi_0, \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger\varphi_0\big) \ = \big(\varphi_0, \hat{a}\big[\hat{a}, \hat{a}^\dagger\hat{a}^\dagger\big]\varphi_0\big) \\ &= \big(\varphi_0, 2\hat{a}\hat{a}^\dagger\varphi_0\big) \ = \big(\varphi_0, \varphi_0\big) \ = 2\,.\end{aligned} \tag{2.17}$$

The properly normalized wavefunction is therefore

$$\varphi_2 \ \equiv \ \frac{1}{\sqrt{2}}\hat{a}^\dagger\hat{a}^\dagger\varphi_0\,. \tag{2.18}$$

We now claim that the n-th excited state of the simple harmonic oscillator is

$$\boxed{\varphi_n \ \equiv \ \frac{1}{\sqrt{n!}}\,\underbrace{\hat{a}^\dagger\cdots\hat{a}^\dagger}_{n}\,\varphi_0 \ = \ \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n\varphi_0\,.} \tag{2.19}$$

Exercise: Verify that this state has $\hat{N}$ eigenvalue n.
Exercise: Verify that the state φ_n is properly normalized.
Since the $\hat{N}$ eigenvalue of φ is n, its energy E_n is given by

$$E_n \ = \ \ \hbar\omega(n + \tfrac{1}{2})\,. \tag{2.20}$$

Since the various states φ_n are eigenstates of a Hermitian operator (the Hamiltonian $\hat{H}$) with different eigenvalues, they are orthonormal

$$\big(\,\varphi_n\,,\,\varphi_m\,\big)\;=\;\delta_{m,n}\,. \tag{2.21}$$

We now note that $\hat{a}\varphi_n$ is a state with $n-1$ operators $\hat{a}^\dagger$ acting on φ_0 because the $\hat{a}$ eliminates one of the creation operators in φ_n. Thus we expect $\hat{a}\varphi_n \sim \varphi_{n-1}$. We can make this precise

$$\hat{a}\,\varphi_n\;=\;\hat{a}\frac{1}{\sqrt{n!}}\big(\hat{a}^\dagger\big)^n\varphi_0\;=\;\frac{1}{\sqrt{n!}}\big[\hat{a}\,,\,\big(\hat{a}^\dagger\big)^n\big]\varphi_0\;=\;\frac{n}{\sqrt{n!}}\big(\hat{a}^\dagger\big)^{n-1}\varphi_0\,. \tag{2.22}$$

At this point we use (2.19) with n set equal to $n-1$ and thus get

$$\hat{a}\,\varphi_n\;=\;\frac{n}{\sqrt{n!}}\sqrt{(n-1)!}\,\varphi_{n-1}\;=\;\sqrt{n}\,\varphi_{n-1}\,. \tag{2.23}$$

By the action of $\hat{a}^\dagger$ on φ_n we get

$$\hat{a}^\dagger\varphi_n\;=\frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^{n+1}\varphi_0\;=\frac{1}{\sqrt{n!}}\sqrt{(n+1)!}\,\varphi_{n+1}\;=\sqrt{n+1}\,\varphi_{n+1}. \tag{2.24}$$

Collecting the results, we have

$$\boxed{\begin{aligned}\hat{a}\,\varphi_n\;&=\;\sqrt{n}\,\varphi_{n-1}\,,\\ \hat{a}^\dagger\varphi_n\;&=\;\sqrt{n+1}\,\varphi_{n+1}\,.\end{aligned}} \tag{2.25}$$

These relations make it clear that $\hat{a}$ lowers the number of any energy eigenstate by one unit, except for the vacuum φ_0 which it kills. The raising operator $\hat{a}^\dagger$ increases the number of any eigenstate by one unit.

Exercise: Calculate the uncertainty Δx of position in the n-th energy eigenstate.

Solution: By definition,

$$(\Delta x)_n^2\;=\;\langle\hat{x}^2\rangle_{\varphi_n}-\langle\hat{x}\rangle_{\varphi_n}^2\,. \tag{2.26}$$

The expectation value $\langle\hat{x}\rangle$ vanishes for any energy eigenstate since we are integrating x, which is odd, against $|\varphi_n(x)|^2$, which is always even. Still, it is instructive to see how this happens explicitly:

$$\langle\hat{x}\rangle_{\varphi_n}\;=\;\big(\varphi_n\,,\hat{x}\varphi_n\big)\;=\;\sqrt{\frac{\hbar}{2m\omega}}\big(\varphi_n\,,\,(\hat{a}+\hat{a}^\dagger)\varphi_n\big)\,, \tag{2.27}$$

using the formula for $\hat{x}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$. The above overlap vanishes because $\hat{a}\varphi_n\sim\varphi_{n-1}$ and $\hat{a}^\dagger\varphi_n\sim\varphi_{n+1}$ and both φ_{n-1} and φ_{n+1} are orthogonal to φ_n. Now we compute the expectation value of $\hat{x}^2$

$$\begin{aligned}\langle\hat{x}^2\rangle_{\varphi_n}\;&=\big(\varphi_n\,,\hat{x}^2\varphi_n\big)\;=\;\frac{\hbar}{2m\omega}\big(\varphi_n\,,\,(\hat{a}+\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger)\varphi_n\big)\\ &=\frac{\hbar}{2m\omega}\big(\varphi_n\,,\,(\hat{a}\hat{a}+\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a}+\hat{a}^\dagger\hat{a}^\dagger)\varphi_n\big)\,.\end{aligned} \tag{2.28}$$

Since $\hat{a}\hat{a}\varphi_n\sim\varphi_{n-2}$ and $\hat{a}^\dagger\hat{a}^\dagger\varphi_n\sim\varphi_{n+2}$ and both φ_{n-2} and φ_{n+2} are orthogonal to φ_n, the $\hat{a}\hat{a}$ and $\hat{a}^\dagger\hat{a}^\dagger$ terms do not contribute. We are left with

$$\langle\hat{x}^2\rangle_{\varphi_n}\;=\;\frac{\hbar}{2m\omega}\big(\varphi_n\,,\,(\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})\varphi_n\big)\,. \tag{2.29}$$

At this point we recognize that $\hat{a}^\dagger \hat{a} = \hat{N}$ and that $\hat{a}\hat{a}^\dagger = [\hat{a}\,, \hat{a}^\dagger] + \hat{a}^\dagger \hat{a} \;= 1 + \hat{N}$. As a result

$$\langle \hat{x}^2 \rangle_{\varphi_n} \;=\; \frac{\hbar}{2m\omega} \big(\varphi_n \,,\, (1 + 2\hat{N}) \varphi_n \big) \;=\; \frac{\hbar}{2m\omega} (1 + 2n) \,. \tag{2.30}$$

We therefore have

$$(\Delta x)_n^2 \;=\; \frac{\hbar}{m\omega} \big(n + \tfrac{1}{2} \big) \,. \tag{2.31}$$

The position uncertainty grows linearly with the number.

Sarah Geller and Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 16: Scattering States and the Step Potential

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April 19, 2016

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1 The Step Potential

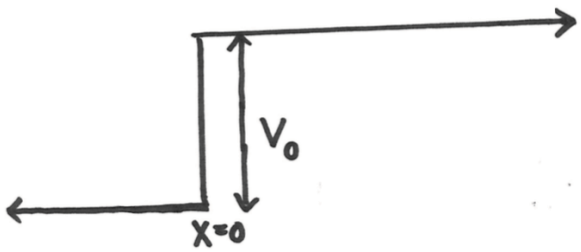

Figure 1: The step potential.

We now begin our detailed study of scattering states. These are un-normalizable energy eigenstates. They simply cannot be normalized, just like momentum eigenstates. These energy eigenstates are not states of particles, one must superpose scattering states to produce normalizable states that can represent a particle undergoing scattering in some potential. Here we examine the step potential (Figure 1), defined by

$$V(x) = \begin{cases} 0\,, & x < 0\,, \\ V_0\,, & x \geq 0\,. \end{cases} \tag{1.1}$$

Our solutions to the Schrödinger equation with this potential will be scattering states of definite energy E. We can consider two cases: $E > V_0$ and $E < V_0$. In both cases the wavefunction extends infinitely to the left and is non-normalizable. Let us begin with the case $E > V_0$.

2 Step Potential with $E > V_0$

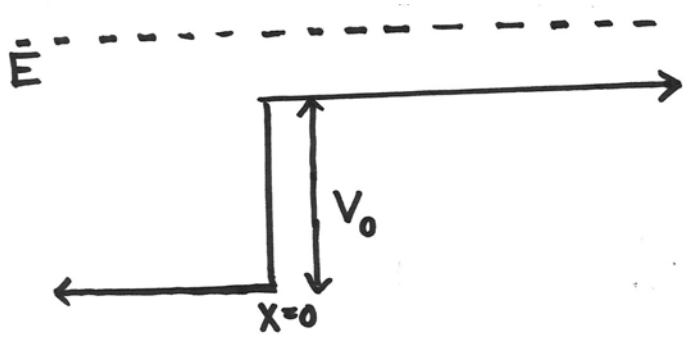

Figure 2: The energy E of the stationary state is greater than the step V_0. The full x axis is classically allowed.

The stationary state with energy E is of the form

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}\,, \tag{2.2}$$

and we will focus first on the unknown $\psi(x)$. In order to write a proper ansatz for $\psi(x)$ we visualize a physical process in which we have a wave incident on the step barrier from the left. Given such a wave traveling in the direction of increasing x, we would expect a reflected wave and a transmitted wave. The reflected wave, moving in the direction of decreasing x, would exist for $x < 0$. The transmitted wave, moving in the direction of increasing x, would exist for $x > 0$. The ansatz for the energy eigenstate must therefore contain all three pieces:

$$\psi(x) = \begin{array}{ll} Ae^{ikx} + Be^{-ikx} & x < 0\,, \\ Ce^{i\bar{k}x} & x > 0\,. \end{array} \tag{2.3}$$

Recall that e^{ikx}, with $k > 0$, represents a wave moving in the direction of increasing x, given the universal time dependence above. Therefore A is the coefficient of the incident wave, B is the coefficient of the reflected wave, and C is the coefficient of the transmitted wave. The waves for $x < 0$ have wavenumber k and the wave for $x > 0$ has wavenumber $\bar{k}$. These wavenumbers are fixed by the Schrödinger equation

$$k^2 \;=\; \frac{2mE}{\hbar^2}\,, \qquad \bar{k}^2 \;=\; \frac{2m(E-V_0)}{\hbar^2}\,. \tag{2.4}$$

There are two equations that constrain our coefficients A, B, and C: both the wavefunction and its derivative must be continuous at $x = 0$. With these two conditions we can solve for B and C in terms of A. This is all we could expect to do: because of linearity the overall scale of these three coefficients must remain undetermined. In fact, we can think of A as the input value and B and C as output values. Let us begin:

- $\psi(x)$ must be continuous at $x = 0$. Thus

$$A + B = C\,. \tag{2.5}$$

- $\psi'(x)$ must be continuous at $x = 0$. Thus

$$ikA - ikB \;=\; i\bar{k}C \quad \rightarrow \quad A - B \;=\; \frac{\bar{k}}{k}\,C\,. \tag{2.6}$$

Solving for B and C in terms of A, we get

$$\boxed{\frac{B}{A} = \frac{k-\bar{k}}{k+\bar{k}}\,, \qquad \frac{C}{A} = \frac{2k}{k+\bar{k}}\,.} \tag{2.7}$$

If A is real B and C are real. For $E = V_0$, we have $\bar{k} = 0$ and equations (2.7) give $B = A$ and $C = 2A$. Therefore, for $E = V_0$ the energy eigenstate is

$$E = V_0 : \qquad \psi(x) = \begin{cases} 2A\cos(kx) & x < 0\,, \\ 2A & x > 0\,, \end{cases} \tag{2.8}$$

and looks like this:

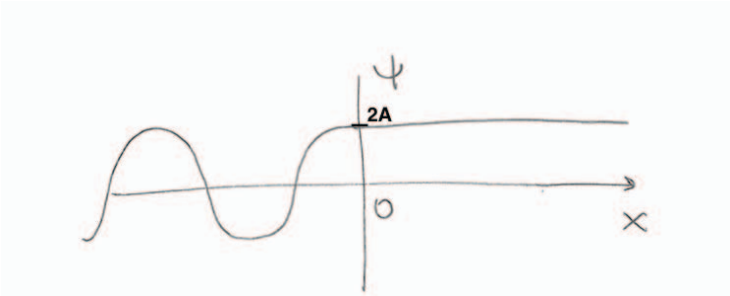

Figure 3: Energy eigenstate for $E = V_0$.

We get further insight into the solution by evaluating the probability current to the left and to the right of the $x = 0$ step. Recall the form of the probability current for a wavefunction ψ is

$$J = \frac{\hbar}{m}\mathrm{Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right) \tag{2.9}$$

A short calculation shows that the current J_L to the left of the step is

$$J_L = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) = J_A - J_B\,, \quad J_A = \frac{\hbar k}{m}|A|^2\,, \quad J_B = \frac{\hbar k}{m}|B|^2\,. \tag{2.10}$$

There is no interference arising from the incident and reflected waves. The total current to the left of the step is simply the current J_A associated with the incident wave minus the current J_B associated with the reflected wave. The current J_R to the right of the step is

$$j_R = \frac{\hbar \bar{k}}{m}\,|C|^2 \;=\; J_C\,. \tag{2.11}$$

In any stationary solution there cannot be accumulation of probability at any region of space because the probability density ρ is manifestly time-independent. While probability is continuously flowing in scattering solutions, it must be conserved. From the conservation equation $\frac{\partial J}{\partial x} + \frac{\partial \rho}{\partial t} = 0$, the time independence of ρ implies that the current J must be x-independent. In particular, our solution (2.7) must imply that $J_L = J_R$. Let us verify this:

$$\begin{aligned} J_L = \;& \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) = \frac{\hbar k}{m}\left(1 - \left(\frac{k-\bar{k}}{k+\bar{k}}\right)^2\right)|A|^2 \\ = \;& \frac{\hbar k}{m}\left(\frac{4k\bar{k}}{(k+\bar{k})^2}\right)|A|^2 = \frac{\hbar \bar{k}}{m}\underbrace{\frac{4k^2}{(k+\bar{k})^2}|A|^2}_{|C|^2} \;=\; \hbar\bar{k}|C|^2 = J_R\,, \end{aligned} \tag{2.12}$$

as expected. The equality of J_L and J_R implies that

$$J_A - J_B = J_C \quad \rightarrow \quad J_A = J_B + J_C \quad \rightarrow \quad 1 = \frac{J_B}{J_A} + \frac{J_C}{J_A}\,. \tag{2.13}$$

We now define the *reflection coefficient* R to be the ratio of the probability flux in the reflected wave to the probability flux in the incoming wave:

$$\boxed{R \;\equiv\; \frac{J_B}{J_A} = \frac{|B|^2}{|A|^2} = \left(\frac{k-\bar{k}}{k+\bar{k}}\right)^2 \leq 1\,.} \tag{2.14}$$

This ratio happens to be the norm squared of the ratio B/A, and it is manifestly less than one, as it should be. We also define the *transmission coefficient* T to be the ratio of the probability flux in the transmitted wave to the probability flux in the incoming wave:

$$\boxed{T \;\equiv\; \frac{J_C}{J_A} = \frac{\bar{k}}{k}\frac{|C|^2}{|A|^2} = \frac{\bar{k}}{k}\frac{4k^2}{(k+\bar{k})^2} = \frac{4k\bar{k}}{(k+\bar{k})^2}\,.} \tag{2.15}$$

The above definitions are sensible because R and T, given in terms of current ratios, add up to one:

$$R + T \;=\; 1\,, \tag{2.16}$$

as follows by inspection of (2.13). Note that $T \neq \frac{|C|^2}{|A|^2}$ because of wavenumbers to the right and to the left of the step are not the same.

Recall that for $E = V_0$ we found $\bar{k} = 0$. In that case we have full reflection: $R = 1$ and $T = 0$. Indeed the probability current associated with the *constant* wavefunction that exists for $x > 0$ (see (2.8)) is zero. Additionally we can give an argument from continuity. The coefficients R and T must be continuous functions of the energy E. For $E < V_0$ we expect $T = 0$ since the forbidden region is all of $x > 0$ and an exponentially decaying wavefuntion cannot carry probability flux. If $T = 0$ for any $E < V_0$ it must still be zero for $E = V_0$, by continuity.

3 Step Potential with $E < V_0$

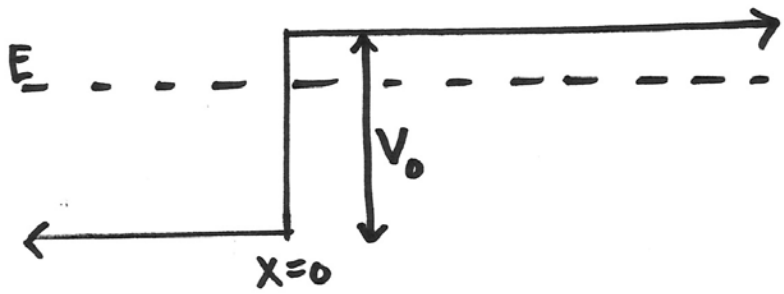

Figure 4: The step potential barrier.

When $E < V_0$ the region $x > 0$ is a classically forbidden region. Let us try to solve for the energy eigenstate without re-doing all the work involved in solving for B and C in terms of A. For this purpose we first note that the ansatz (2.3) for $x < 0$ can be left unchanged. On the other hand, for $x > 0$ the earlier solution

$$\psi(x) \;=\; Ce^{i\bar{k}x}\,, \qquad k^2 \;=\; \frac{2m(E-V_0)}{\hbar^2}\,, \tag{3.17}$$

should become a decaying exponential

$$\psi(x) \;=\; Ce^{-\kappa x}\,, \qquad \kappa^2 \;=\; \frac{2m(V_0-E)}{\hbar^2}\,. \tag{3.18}$$

We note that the former becomes the latter upon the replacement

$$\bar{k} \;\to\; i\,\kappa\,. \tag{3.19}$$

This means that we can simply perform this replacement in our earlier expressions for B/A and C/A and we obtain the new expressions. In particular from (2.7) we get

$$\frac{B}{A} = \frac{k-i\kappa}{k+i\kappa} \tag{3.20}$$

Therefore

$$\frac{B}{A} = \frac{i(k-i\kappa)}{i(k+i\kappa)} = -\frac{\kappa+ik}{\kappa-ik} \;=\; -\,e^{2i\delta(E)}\,, \tag{3.21}$$

with

$$\boxed{\delta(E) = \tan^{-1}\Big(\frac{k}{\kappa}\Big) = \tan^{-1}\Big(\sqrt{\frac{E}{V_0-E}}\Big)\,.} \tag{3.22}$$

Since the magnitude of A is equal to the magnitude of B, we have $J_A = J_B$ and $J_C = 0$. Thus $T = 0$ and $R = 1$. As noted above, the ratio B/A is a pure phase. The phase of the numerator $\kappa + ik$ is $\delta(E)$ and the phase of the denominator $\kappa - ik$ is $-\delta(E)$, thus the total phase $2\delta(E)$ for the ratio. We did not absorb the minus sign into the phase; in this way $\delta(E) \to 0$ as $E \to 0$. Note that $\delta(E)$ is positive and does not exceed $\pi/2$. In fact a sketch of $\delta(E)$ is given in Figure 5.

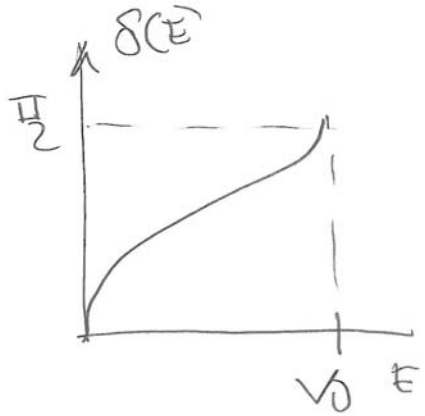

Figure 5: The phase $\delta(E)$ as a function of energy $E < V_0$.

The total wavefunction for $x < 0$ is interesting

$$\begin{aligned}\psi(x) \;&=\; Ae^{ikx} + (-Ae^{2i\delta(E)})e^{-ikx} \\ &=\; Ae^{i\delta(E)}\big(e^{-i\delta(E)}e^{ikx} - e^{i\delta(E)}e^{-ikx}\big) \\ &=\; 2iAe^{i\delta(E)}\sin(kx-\delta(E))\end{aligned} \tag{3.23}$$

This means that the probability density is

$$|\psi|^2 \;=\; 4A^2\sin^2(kx-\delta(E))\,. \tag{3.24}$$

The point $x_0 > 0$ determined by the condition $kx_0 = \delta(E)$ is the point in the forbidden region where the extrapolation of the allowed-region solution would vanish. Of course in the forbidden region $x > 0$, the probability density $|\psi|^2$ is a decaying exponential.

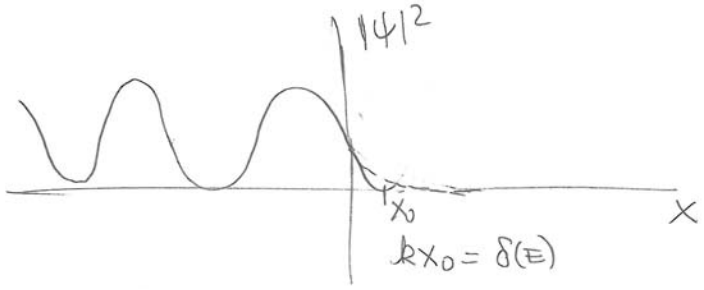

Figure 6: Norm squared for the energy eigenstate when $E < V_0$. For $x > 0$ the probability density decays exponentially with x. The point x_0 is the point where the extrapolation of the $x < 0$ probability density would have vanished.

For future use we record the derivative of the phase $\delta(E)$ with respect to the energy

$$\delta'(E) \equiv \frac{d\delta(E)}{dE} = \frac{1}{2}\sqrt{\frac{1}{E(V_0 - E)}}\,. \tag{3.25}$$

Note that this derivative becomes infinite both for $E \to 0$ and for $E \to V_0$.

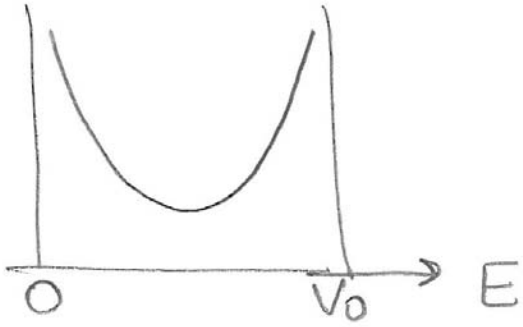

Figure 7: The derivative $\delta'(E)$ as a function of energy $E < V_0$.

4 Wavepackets in the step potential

Now we examine the more physical scenario. As we've seen with the free particle, the stationary states are not normalizable, and physical particles are actually represented by wavepackets built with an infinite superposition of momentum eigenstates. We can do similarly thing with our energy eigenstates. We will consider energy eigenstates with $E > V_0$ or equivalently with $k^2 > \hat{k}^2$, where

$$k^2 = \frac{2mE}{\hbar^2} > \frac{2mV_0}{\hbar^2} \equiv \hat{k}^2\,, \tag{4.26}$$

and we will superpose them. To begin we write the energy eigenstates in a slightly different form, including the time dependence. Setting $A = 1$ and using the values for the ratios B/A and C/A we find the solution

$$\Psi(x,t) = \begin{cases} \left(e^{ikx} + \frac{k-\bar{k}}{k+\bar{k}}\, e^{-ikx}\right) e^{-iE(k)t/\hbar}\,, & x < 0\,, \\ \frac{2k}{k+\bar{k}}\, e^{i\bar{k}x}\, e^{-iE(k)t/\hbar}\,, & x > 0\,. \end{cases} \tag{4.27}$$

We can form a superposition of these solutions by multiplying by a function $f(k)$ and integrating over k

$$\Psi(x,t) = \begin{cases} \int_{\hat{k}}^{\infty} dk\, f(k) \left(e^{ikx} + \frac{k-\bar{k}}{k+\bar{k}}\, e^{-ikx} \right) e^{-iE(k)t/\hbar}\,, & x<0\,, \\ \int_{\hat{k}}^{\infty} dk\, f(k)\, \frac{2k}{k+\bar{k}}\, e^{i\bar{k}x}\, e^{-iE(k)t/\hbar}\,, & x>0\,. \end{cases} \tag{4.28}$$

Here $f(k)$ is a real function of k that is essentially zero except for a narrow peak at $k=k_0$. Note that we have only included momentum components with energy greater than V_0 by having the integral's lower limit set equal to $\hat{k}$. The integral only runs over positive k because only in that case the e^{ikx} waves are moving towards positive x, and are therefore genuine incident waves. The above is guaranteed to be a solution of the Schrödinger equation.

We can split the solution into incident, reflected and transmitted waves, as follows.

$$\Psi(x,t) = \begin{cases} \Psi_{inc}(x,t) + \Psi_{ref}(x,t)\,, & x<0\,, \\ \Psi_{trans}(x,t)\,, & x>0\,. \end{cases} \tag{4.29}$$

Naturally both $\Psi_{inc}(x,t)$ and $\Psi_{ref}(x,t)$ exist for $x<0$ and $\Psi_{trans}(x,t)$ exists for $x>0$. We then have, explicitly

$$\begin{aligned} \Psi_{inc}(x<0,t) &= \int_{\hat{k}}^{\infty} dk\, f(k) e^{ikx} e^{-iE(k)t/\hbar}\,, \\ \Psi_{ref}(x<0,t) &= \int_{\hat{k}}^{\infty} dk\, f(k) \left(\frac{k-\bar{k}}{k+\bar{k}} \right) e^{-ikx} e^{-iE(k)t/\hbar}\,, \\ \Psi_{trans}(x>0,t) &= \int_{\hat{k}}^{\infty} d\bar{k}\, f(\bar{k}) \left(\frac{2k}{k+\bar{k}} \right) e^{i\bar{k}x} e^{-iE(k)t/\hbar}\,. \end{aligned} \tag{4.30}$$

How does the peak of $\Psi_{inc}(x,t)$ move? For this we look for the main contribution to the associated integral which occurs when the total phase in the integrand is stationary for $k \approx k_0$. We therefore require

$$\frac{d}{dk} \left(kx - \frac{\hbar^2 k^2}{2m} \frac{t}{\hbar} \right) \Big|_{k_0} = 0 \quad \to \quad x - \frac{\hbar k_0}{m} t = 0 \quad \Longrightarrow \quad x = \frac{\hbar k_0}{m}\, t\,. \tag{4.31}$$

This is the relation between t and x satisfied by the peak of Ψ_{inc}. It describes a peak moving with constant velocity $\hbar k_0/m > 0$. Since $\Psi_{inc}(x,t)$ requires that $x<0$, the above condition shows that we get the peak only for $t<0$. The peak of the packet gets to $x=0$ at $t=0$. For $t>0$, $\Psi_{inc}(x,t)$ is not zero, but it must be rather small, since the stationary phase condition cannot be satisfied for any x in the domain $x<0$.

Consider now $\Psi_{ref}(x,t)$. This time the stationary phase condition is

$$\frac{d}{dk} \Big(-kx - \frac{\hbar^2 k^2}{2m} \frac{t}{\hbar} \Big) \Big|_{k_0} = 0 \quad \to \quad x + \frac{\hbar k_0}{m} t = 0 \quad \Longrightarrow \quad x = -\frac{\hbar k_0}{m}\, t\,. \tag{4.32}$$

The relation represents a peak moving with constant negative velocity $-\hbar k_0/m$. Since $\Psi_{ref}(x,t)$ requires that $x<0$, the above condition shows that we get the peak only for $t>0$, as it befits a reflected wave. For $t>0$, $\Psi_{ref}(x,t)$ is not zero, but it must be rather small, since the stationary phase condition cannot be satisfied for any x in the domain $x<0$.

Finally, let us consider Ψ_{trans}. The stationary phase condition reads:

$$\frac{d}{dk}\left(\bar{k}x - \frac{\hbar^2 k^2}{2m}\frac{t}{\hbar}\right)\Big|_{k_0} = 0 \quad \rightarrow \quad \frac{d\bar{k}}{dk}\Big|_{k_0} x - \frac{\hbar k_0}{m}t = 0 \tag{4.33}$$

Using

$$\bar{k}^2 \;=\; k^2 - \frac{2mV_0}{\hbar^2} \quad \rightarrow \quad \frac{d\bar{k}}{dk} = \frac{k}{\bar{k}}\,, \tag{4.34}$$

back to the earlier equation we quickly find that

$$\text{Transmitted wave peak:} \quad x \;=\; \frac{\hbar\bar{k}}{m}\,t\,, \tag{4.35}$$

with $\bar{k}$ evaluated for $k = k_0$. Since $x > 0$ is the domain of Ψ_{trans} this describes a peak moving to the right with velocity $\hbar\bar{k}/m$ for $t > 0$. For $t < 0$, $\Psi_{trans}(x,t)$ is not zero, but it must be rather small, since the stationary phase condition cannot be satisfied for any x in the domain $x > 0$.

In summary, for large negative time Ψ_{inc} dominates and both Ψ_{ref} and Ψ_{trans} are very small. For large positive time, both Ψ_{ref} and Ψ_{trans} dominate and Ψ_{inc} becomes very small. These situations are sketched in figures 8 and 9. Of course for small times, positive or negative, all three waves exist and together they describe the complex process of collision with the step in which a reflected and a transmitted wave are generated.

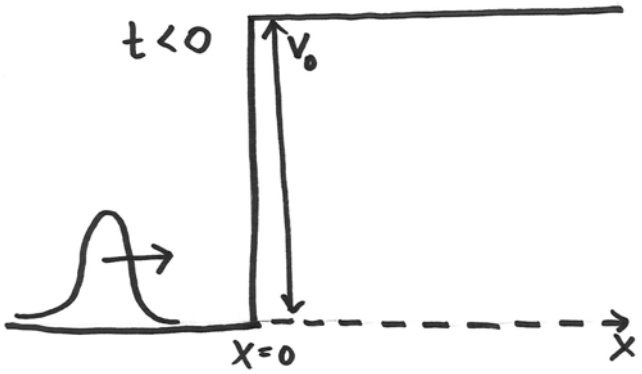

Figure 8: At large negative times an incoming wavepacket is traveling in the $+x$ direction.

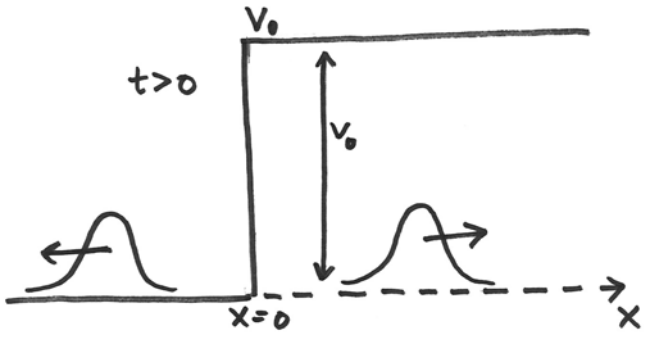

Figure 9: At large positive times we have a reflected wavepacket traveling in the $-\hat{x}$ direction and the transmitted wavepacket traveling in the $+\hat{x}$ direction.

Let us now examine a wavepacket built with energies $E < V_0$. Recall that in this situation $B/A = -e^{2i\delta(E)}$. Therefore for an incident wave, all of whose momentum components have energy less

than V_0,

$$\Psi_{inc}(x<0,t) \;=\; \int_0^{\hat{k}} dk\, f(k)\, e^{ikx} e^{-iEt/\hbar}\,, \tag{4.36}$$

the associated reflected wavefunction is

$$\Psi_{ref}(x<0,t) \;=\; -\int_0^{\hat{k}} dk\, f(k)\, e^{2i\delta(E)} e^{-ikx} e^{-iEt/\hbar}\,. \tag{4.37}$$

Using the method of stationary phase again to find the evolution of the peak,

$$\frac{d}{dk}\left(2\delta(E) - kx - \frac{Et}{\hbar}\right)\bigg|_{k_0} = 0 \quad \rightarrow \quad 2\delta'(E)\frac{\hbar^2 k_0}{m} - x - \frac{\hbar k_0 t}{m} \;=\; 0\,. \tag{4.38}$$

From this we quickly find

$$x \;=\; -\frac{\hbar k_0}{m}\left(t - 2\hbar\,\delta'(E)\right), \tag{4.39}$$

where the derivative is evaluated at $E(k_0)$. The reflected wave packet is moving towards more negative x as time grows positive. This is as it should. But there is a time delay associated with the reflected packet, evident when we compare the above equation with $x = -\frac{\hbar k_0}{m} t$. The time delay is given by

$$\boxed{\text{time delay} \;=\; 2\hbar\,\delta'(E)\,.} \tag{4.40}$$

The derivative $\delta'(E)$ was evaluated in (3.25) and it is positive. We see that the delay is particularly large for wave packets of little energy or those with energies just below V_0.

We conclude the analysis of the step potential by discussing what it means to observe the particle in the forbidden region. It would be contradictory if the observer could make the following two statements:

1. The particle is located in the forbidden region.
2. The particle has energy less than V_0.

Both statements taken to hold simultaneously would imply that the particle has negative kinetic energy, something that is inconsistent. In particular with $E < V_0$ we would have a negative kinetic of magnitude $V_0 - E$.

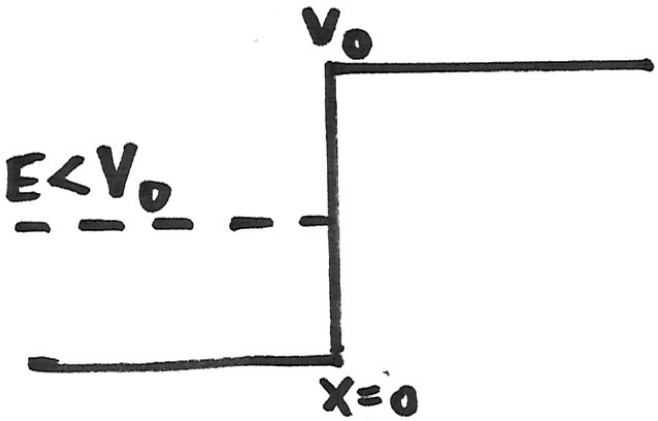

Figure 10: The step potential with potential energy V_0. If we could observe a particle in the forbidden region with energy E then the kinetic energy would be negative.

First note that in the solution the particle penetrates into the forbidden region a distance of about $1/\kappa$, where, you will recall that

$$\kappa^2 = \frac{2m(V_0 - E)}{\hbar^2}\,. \tag{4.41}$$

To be sure the particle is in the forbidden region its position uncertainty Δx must be smaller than the penetration depth:

$$\Delta x \leq \frac{1}{\kappa}\,. \tag{4.42}$$

The particle acquires some momentum p due to the position measurement:

$$p \geq \frac{\hbar}{\Delta x} \;\geq\; \hbar\kappa\,. \tag{4.43}$$

Due to this momentum induced by the position measurement there is some additional contribution E' to the kinetic energy

$$E' \;=\; \frac{p^2}{2m} \;\geq\; \frac{\hbar^2\kappa^2}{2m} = V_0 - E\,, \tag{4.44}$$

where we used (4.41). From this inequality we find that the total energy will exceed V_0

$$E_{tot} \;=\; E + E' \geq E + (V_0 - E) = \; V_0\,. \tag{4.45}$$

While the argument is heuristic, it gives some evidence that no negative kinetic energy will be detected for a particle that is found in the forbidden region.

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Chapter 17: Resonant transmission and Ramsauer–Townsend

B. Zwiebach
April 26, 2016

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1 Resonant transmission in a square well **1**

2 The Ramsauer–Townsend Effect **3**

1 Resonant transmission in a square well

Consider the finite square well

$$V(x) \;= \begin{cases} 0\,, & \text{for} \quad |x| > a\,, \\ -V_0\,, & \text{for} \quad |x| < a\,. \end{cases} \tag{1.1}$$

Here $V_0 > 0$ has units of energy. We consider an energy eigenstate, a scattering solution with $E > 0$ that represents an incoming wavefunction approaching the well from the left. An ansatz for the eigenstate will be of the form

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ Ce^{ik_2 x} + De^{-ik_2 x}\,, & |x| < a \\ Fe^{ikx}\,, & x > a\,. \end{cases} \quad , \tag{1.2}$$

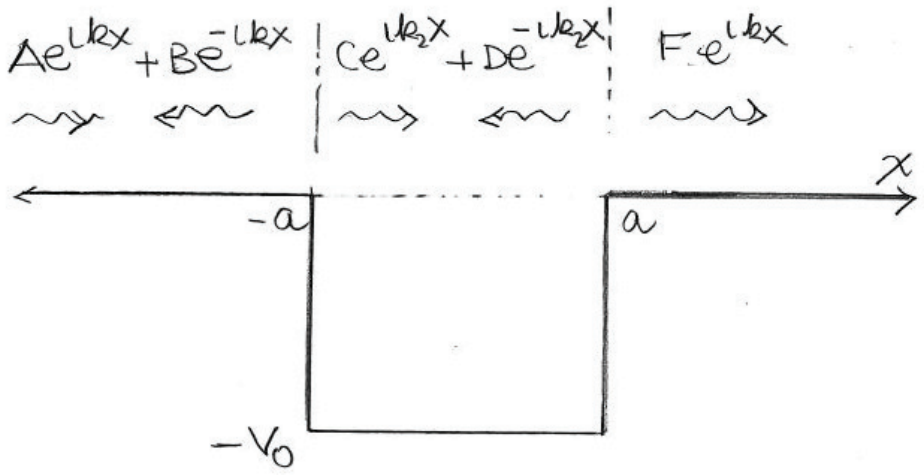

Figure 1: The square well with all the relevant waves as one, with coefficient A is incident from the left.

Here A is the coefficient of the incoming wave that exists for $x < a$, and B is the coefficient of the reflected wave (see Figure 1). Both of these waves have wavenumber k. In the well region $|x| < a$ we have a wave moving to the right, with coefficient C and a wave moving to the left, with coefficient D. The wavenumber in this region is called k_2. To the right of the well we have just one wave, moving

to the right. Its coefficient is F and its wavenumber k. Note that even though the potential is an even function of x, a non-normalizable energy eigenstate need not be even nor odd. The symmetry is broken by the condition that a wave is incident from the left. The values of k and k', both positive, are determined by the Schrödinger equation and are

$$k^2 \;=\; \frac{2mE}{\hbar^2}\,, \quad k_2^2 \;=\; \frac{2m(E+V_0)}{\hbar^2}\,. \tag{1.3}$$

There are four boundary conditions: continuity of ψ and ψ' at $x=-a$ and at $x=a$. These four equations can be used to fix the coefficients B, C, D, and F in terms of A. We define reflection and transmission coefficients R and T as follow

$$R \;\equiv\; \frac{|B|^2}{|A|^2}\,, \quad T \;\equiv\; \frac{|F|^2}{|A|^2}\,. \tag{1.4}$$

From probability current conservation we know that the currents to the left and to the right of the well must be equal so that

$$|A|^2 - |B|^2 = |F|^2\,. \tag{1.5}$$

This is not an independent equation; it must follow from the boundary conditions. It implies that

$$R+T = \frac{|B|^2}{|A|^2} + \frac{|F|^2}{|A|^2} = 1\,, \tag{1.6}$$

showing that our definition of R and T makes sense.

Solving for R and T is straightforward but a little laborious. Let us just quote the answer that one gets. The transmission coefficient is the following function of the energy E of the eigenstate:

$$\frac{1}{T} \;=\; 1 \,+\, \frac{1}{4}\frac{V_0^2}{E(E+V_0)}\sin^2(2k_2a). \tag{1.7}$$

Since the second term in the right-hand side is manifestly positive, we have $T \le 1$. As $E \to 0$, we have $\frac{1}{T} \to 1+\infty$, which means $T \to 0$. As $E \to \infty$, we have $T \to 1$.

We can remove all units from this result by defining

$$e \;\equiv\; \frac{E}{V_0}\,, \quad z_0^2 \;\equiv\; \frac{2ma^2V_0}{\hbar^2}\,. \tag{1.8}$$

Then,

$$(k_2a)^2 \;=\; \frac{2ma^2(E+V_0)}{\hbar^2} \;=\; \frac{2ma^2V_0}{\hbar^2}(1+e) \quad\to\quad 2k_2a = 2z_0\sqrt{1+e}, \tag{1.9}$$

so we have

$$\boxed{\frac{1}{T} \;=\; 1 + \frac{1}{4e(1+e)}\sin^2(2z_0\sqrt{1+e})\,.} \tag{1.10}$$

We now can see that the well becomes transparent, making $T=1$, for certain values of the energy. All we need is that the argument of the sin function be a multiple of π:

$$2z_0\sqrt{1+e} \;=\; n\pi, \quad n \in \mathbb{Z}. \tag{1.11}$$

Not all integers are allowed. Because $e > 0$, the left-hand side is bigger than or equal to $2z_0$ and therefore

$$n \ge \frac{2z_0}{\pi}. \tag{1.12}$$

Call the associated energies $E_n = e_n V_0$. Then

$$e_n + 1 \;=\; \frac{n^2\pi^2}{4z_0^2} \;=\; \frac{n^2\pi^2\hbar^2}{2m(2a)^2V_0}\,, \tag{1.13}$$

so that

$$E_n + V_0 \;=\; \frac{n^2\pi^2\hbar^2}{2m(2a)^2}\,. \tag{1.14}$$

Note that $E_n + V_0$ is the energy of the scattering state measured with respect to the bottom of the square well. The right-hand side is the energy of the n-th bound state of the *infinite* square well of width $2a$. We thus have a rather surprising result: *We get full transmission for those energies $E_n > 0$ that are in the spectrum of the infinite-square-well extension of our finite square well.* The inequality $n \geq \frac{2z_0}{\pi}$ guarantees that $E_n > 0$. Since infinite square well bound states are characterized by fitting an integer number of half wavelengths, we have a resonance type situation in which perfect transmission is happening when the scattering waves fit perfectly inside the *finite* square well. The phenomenon we have observed is called resonant transmission!

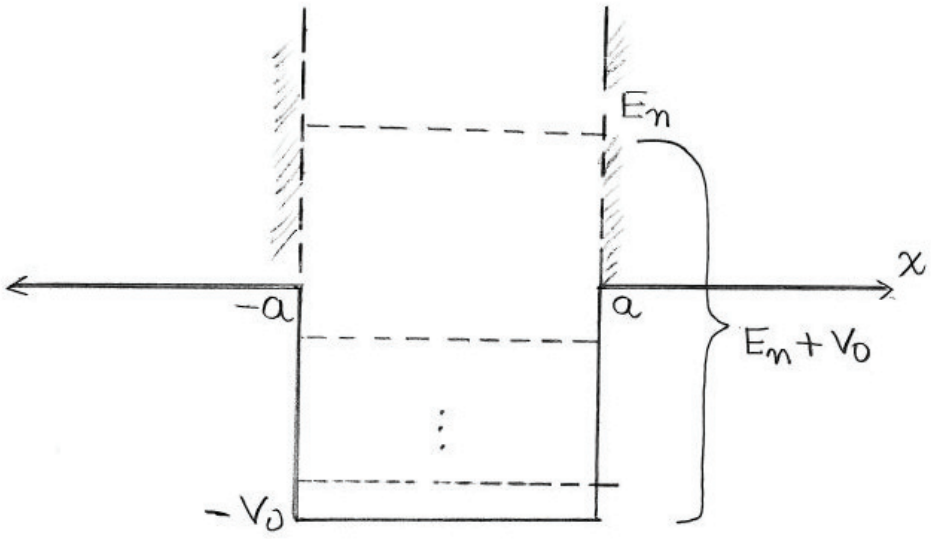

Figure 2: We get resonant transmission across the finite well at the positive bound-state energies of a would-be infinite well.

The fitting of an exact number of half wavelengths can also be seen directly from the vanishing of the sin function in (1.7) giving $k_2(2a) = n\pi$ which implies

$$\frac{2\pi}{\lambda}(2a) \;=\; n\pi \quad\rightarrow\quad 2a \;=\; n\,\tfrac{\lambda}{2}\,. \tag{1.15}$$

We show in Figure 3 the transmission coefficient T as a function of $e = E/V_0$ for a square well with $z_0 = 13\pi/4$. In this case we must have $n \geq \frac{13}{2}$ or $n \geq 7$.

2 The Ramsauer–Townsend Effect

Carl Ramsauer and John Sealy Townsend published separately their investigations in 1921. They were studying the elastic scattering of low-energy electrons off of rare-gas atoms, such as noble gases.

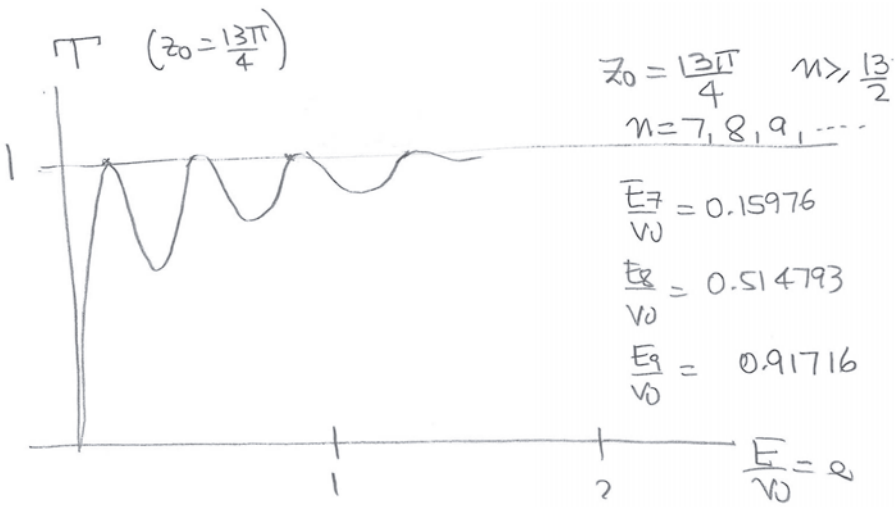

Figure 3: The transmission coefficient T as a function of e for a square well with $z_0 = \frac{13\pi}{4}$. At the energies for which $T = 1$ we have resonant scattering. The values of $E_7, E_8, \ldots$ are indicated in the figure. There are three cases of resonant transmission for $0 < E < V_0$. Note that the spacing between the points where $T = 1$ grows as e grows.

These gases have their electronic shells fully filled and are both very un-reactive and have high ionization energies. The potential is created by the nucleus, and becomes visible as the incident electron penetrates the electron cloud. This potential is a spherically symmetric attractive potential for the electrons – some kind of finite spherical well. In the experiment some electrons collide with the atoms and scatter, mostly bouncing back. We can thus view the reflection coefficient R as a proxy for the scattering cross section!

Ramsauer and Townsend reported a very unusual phenomenon. At very low energies, the scattering cross section was high. But the energy dependence was surprising. As the energy was increased the scattering went down towards zero, to go up again as the energy was increased further. Such mysterious behavior had no sensible classical explanation. What one has at play is quantum-mechanical resonant scattering. The cross section going to zero means the reflection coefficient going to zero, and the transmission coefficient going to one! The first resonant transmission happens for electrons of around one electron-volt (such electrons have a speed of about 600 Km/s). Figure 4 provides a sketch of both R and T as a function of energy. Our one-dimensional square well potential does not provide a good quantitative match for the data, but it illustrates the physical phenomenon. A three-dimensional spherical square well is needed for a quantitative analysis.

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

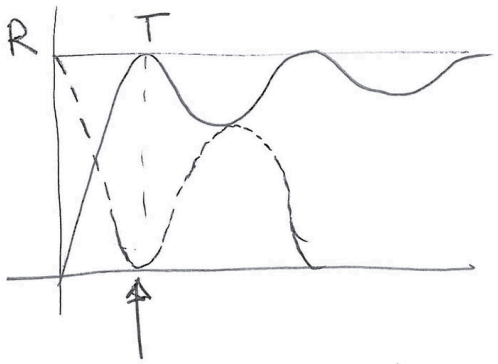

Figure 4: The reflection and transmission coefficients as a function of energy for the Ramsauer–Townsend effect. Note that $R + T = 1$. At the arrow, we have $R = 0$, so there is no scattering. All of the electrons go straight through the noble gas atoms! They experience resonant transmission. This first occurs around 1eV.

Chapter 18: Scattering in one dimension

B. Zwiebach
April 26, 2016

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1 Scattering in One Dimension

Physicists learn a lot from scattering experiments. Rutherford learned about the structure of the atom by scattering alpha particles off thin layers of gold. We have *elastic* scattering if particles do not change type; this typically requires low energies. At high energies, scattering becomes quite complicated due to the creation of new particles.

The scattering of a particle off a fixed target is studied by working with a particle moving in a potential, the potential created by the target. Even in the case of particle *collisions* it is generally possible to study the problem using center of mass coordinates and, again, considering scattering in a potential.

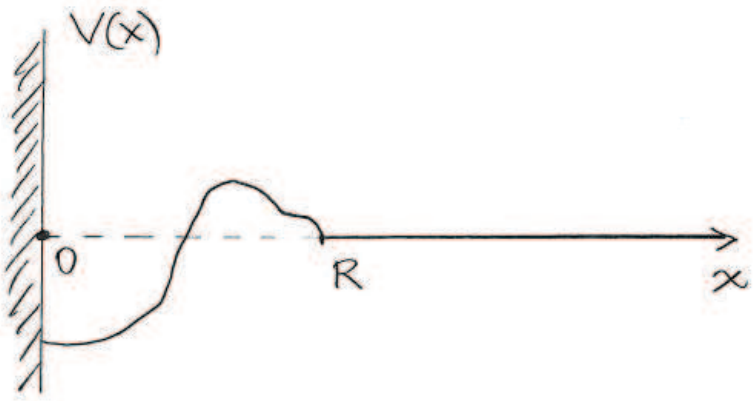

Figure 1: A potential of range R. The potential vanishes for $x > R$ and is infinite for $x \leq 0$.

We consider (elastic) scattering in the general potential shown in Fig. 3. This potential is given by

$$V(x) = \begin{cases} \mathcal{V}(x) & 0 < x < R\,, \\ 0 & x > R\,, \\ \infty & x < 0\,. \end{cases} \tag{1.1}$$

We call this a *finite range* potential, because the nontrivial part $\mathcal{V}(x)$ of the potential does not extend beyond a distance R from the origin. Moreover, we have an infinite potential wall at $x = 0$. Thus all the physics happens in $x > 0$ and incoming waves from $x \to \infty$ will be eventually reflected back, giving the physicist information about the potential. The restriction to $x > 0$ will also be useful when

we later study the more physical case of scattering in three dimensions. In that case, when using spherical coordinates, we have $r > 0$ and most of the concepts to be learned here will apply.

Consider first the case where $\mathcal{V}(x) = 0$, so that

$$V(x) = \begin{cases} 0 & x > 0\,, \\ \infty & x < 0\,, \end{cases} \tag{1.2}$$

as shown in figure 2. We have a free particle, except for the wall at $x = 0$. The solutions can be constructed using linear combination of momentum eigenstates $e^{\pm ikx}$ where

$$k^2 \;=\; \frac{2mE}{\hbar^2}\,. \tag{1.3}$$

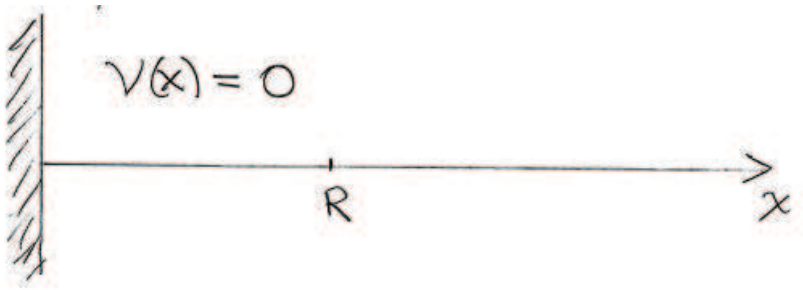

Figure 2: The zero potential and its energy eigenstates $\phi(x) = \sin kx$ are needed to compare with the $\mathcal{V}(x) \neq 0$ problem.

The solution has an incoming wave e^{-ikx} and an outgoing wave e^{ikx} combined in such a way that $\phi(0) = 0$ as required by the presence of the wall:

$$\phi(x) \sim e^{ikx} - e^{-ikx}. \tag{1.4}$$

Better yet, we can divide this solution by $2i$ to find

$$\boxed{\phi(x) \;=\; -\frac{e^{-ikx}}{2i} + \frac{e^{ikx}}{2i} \;=\; \sin kx\,.} \tag{1.5}$$

The incoming wave is the first term to the right of the first equal sign and the reflected wave is the second term. Both carry the same amount of probability flux, but in opposite directions.

Now consider the case $\mathcal{V}(x) \neq 0$. This potential always acts over the finite range $0 < x < R$ and we will eventually be interested in computing the energy eigenstate wavefunction $\psi(x)$ in this region. For the moment, however, let us consider $\psi(x)$ in the region $x > R$. We will take the incoming wave to be the same one we had for the zero-potential solution $\phi(x)$:

$$\text{Incoming wave:} \qquad -\frac{e^{-ikx}}{2i} \tag{1.6}$$

The outgoing wave to be added to the above requires an e^{ikx}, to have the same energy as the incoming wave solution. We now claim that the most general solution includes a phase factor, so we have

$$\text{Outgoing wave:} \qquad e^{2i\delta}\,\frac{e^{ikx}}{2i}\,, \quad \delta \in \mathbb{R}\,. \tag{1.7}$$

We note that the phase δ cannot be a function of x: the free Schrödinger equation for $x > R$ only allows phases linear in x, but that would change the value of the momentum associated with the outgoing wave, which we have already argued must be k. Furthermore, δ cannot be complex because then we would fail to have equality between incident and reflected probability fluxes. This condition requires that the norm-squared of the numbers multiplying the exponentials $e^{\pm ikx}$ be the same. Thus, δ is a real function that depends on the energy E of the eigenstate and, of course, of the potential $V(x)$. A natural range of δ is from zero to 2π, but it will be easier to let it range through all of the reals $\mathbb{R}$ in order to achieve a δ that is a *continuous* function of the energy. Assembling together the incident and reflected components of the $x > R$ solution we get

$$\boxed{\psi(x) \;=\; \tfrac{1}{2i}\big(-e^{-ikx} + e^{ikx+2i\delta}\big) \;=\; e^{i\delta}\sin(kx+\delta)\,, \quad \text{for} \quad x > R\,.} \tag{1.8}$$

This is called the *canonical solution* for $x > R$. For any particular feature of the solution $\phi(x)$ that we might find at $kx = a_0$, giving $x = a_0/k$, we would find the same feature in $\psi(x)$ at $k\tilde{x} + \delta = a_0$, giving $\tilde{x} = a_0/k - \delta/k$. For small $\delta > 0$, the wave is *pulled in* by an amount δ/k, and the potential is exerting attraction. For small $\delta < 0$, the wave is pushed out by an amount $|\delta|/k$, and the potential is exerting repulsion. Note also that δ and $\delta \pm \pi$ give exactly the same $\psi(x)$. This is simplest to see from the first form in (1.8).

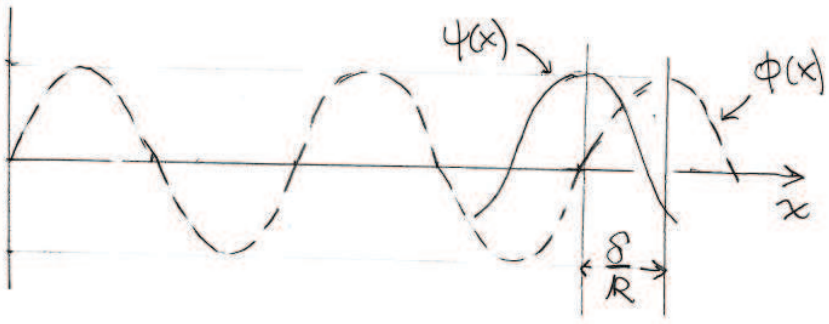

Figure 3: The solution $\phi(x)$ for zero potential is shown with a dashed line. For $x > R$, the solution $\psi(x)$is shown as a continuous line. As compared to $\phi(x)$, it is spatially shifted towards the origin by a distance δ/k.

We define the *scattered wave* $\psi_s(x)$ as the extra wave in the solution $\psi(x)$ that would vanish for the case of zero potential, i.e.

$$\psi(x) = \phi(x) + \psi_s(x). \tag{1.9}$$

Note that both ϕ and ψ have the same incident wave, so ψ_s must be an outgoing wave. We find, indeed

$$\psi_s(x) = \;\psi(x) - \phi(x) \;=\; -\frac{e^{-ikx}}{2i} + \frac{e^{ikx+2i\delta}}{2i} + \frac{e^{-ikx}}{2i} - \frac{e^{ikx}}{2i} \;=\; \frac{e^{ikx+2i\delta}}{2i} - \frac{e^{ikx}}{2i}\,, \tag{1.10}$$

and therefore we get

$$\psi_s(x) \;=\; e^{i\delta}\sin\delta\, e^{ikx} \;=\; A_s e^{ikx}, \quad \text{with} \quad A_s \;\equiv\; e^{i\delta}\sin\delta\,. \tag{1.11}$$

A_s is called the *scattering amplitude*, being the amplitude for the scattered wave. While we can't normalize our states yet (for that we need wave packets) the probability to scatter is captured by

$$|A_s|^2 = \sin^2\delta. \tag{1.12}$$

1.1 Time Delay

The quantity $\delta(E)$ determines the time delay of a reflected wave packet, as compared to a wave packet that would encounter a zero potential. Indeed we claim that the delay is given by

$$\Delta t \;=\; 2\hbar\,\delta'(E)\,, \tag{1.13}$$

where prime denotes derivative with respect to the argument, and the evaluation is done for the central energy of the superposition that builds the wave packet. If $\Delta t < 0$, then the particle spends less time near $x = 0$, either because the potential is attractive and the particle speeds up, or because the potential is repulsive and the particle bounces before reaching $x = 0$. If $\Delta t > 0$, then the particle spends more time near $x = 0$, typically because it slows down or gets temporarily trapped in the potential.

We write the incoming wave in the form

$$\psi_{\rm inc}(x,t) = \int_0^\infty dk\; g(k) e^{-ikx} e^{-iE(k)t/\hbar}, \quad x > R\,, \tag{1.14}$$

where $g(k)$ is a real function peaked around $k = k_0$. We write the associated reflected wave by noticing that the above is a superposition of waves as in (1.6) and the reflected wave must be the associated superposition of waves as in (1.7). We must therefore change the sign of the momentum, change the overall sign and multiply by the phase $e^{2i\delta}$:

$$\psi_{\rm refl}(x,t) = -\int_0^\infty dk\; g(k) e^{ikx} e^{2i\delta(k)} e^{-iE(k)t/\hbar}\,, \quad x > R\,. \tag{1.15}$$

We now use the stationary phase approximation to figure out the motion of the wave packet peak. We must have a stationary phase when $k = k_0$:

$$\begin{aligned} 0 &= \frac{d}{dk}\left(kx + 2\delta(k) - \frac{E(k)t}{\hbar}\right)\Big|_{k_0} \\ &= x + 2\,\frac{d\delta}{dk}\Big|_{k_0} - \frac{dE}{dk}\Big|_{k_0}\frac{t}{\hbar} \\ &= x + 2\,\frac{dE}{dk}\Big|_{k_0}\frac{d\delta}{dE}\Big|_{E(k_0)} - \frac{dE}{dk}\Big|_{k_0}\frac{t}{\hbar} \\ &= x + \frac{1}{\hbar}\,\frac{dE}{dk}\Big|_{k=k_0}\Big(2\hbar\,\frac{d\delta}{dE}\Big|_{E(k_0)} - t\Big) \\ &= x + \frac{\hbar k_0}{m}\Big(2\hbar\,\frac{d\delta}{dE}\Big|_{E(k_0)} - t\Big), \end{aligned} \tag{1.16}$$

giving

$$x \;=\; \frac{\hbar k_0}{m}\Big(t - 2\hbar\,\frac{d\delta}{dE}\Big|_{E(k_0)}\Big)\,. \tag{1.17}$$

Here $\hbar k_0/m$ is the familiar group velocity v_0 of the wavepacket. If there had been no phase shift δ, say because $\mathcal{V}(x) = 0$, there would be no time delay and the peak of the reflected wavepacket would follow the line $x = v_0 t$. Therefore the delay, as claimed, is given by

$$\Delta t \;=\; 2\hbar\,\delta'(E(k_0))\,. \tag{1.18}$$

We can compare the time delay to a natural time in the problem. We first rewrite

$$\Delta t \;=\; 2\hbar \frac{dk}{dE}\frac{d\delta}{dk} \;=\; \frac{2}{\left(\frac{1}{\hbar}\frac{dE}{dk}\right)}\frac{d\delta}{dk}\,. \tag{1.19}$$

We know that

$$\frac{1}{\hbar}\frac{dE}{dk} = \frac{d\omega}{dk} = v_0, \tag{1.20}$$

so we can then write

$$\frac{d\delta}{dk} = \frac{\Delta t}{2} v_0. \tag{1.21}$$

Multiplying this by $\frac{1}{R}$, we have

$$\boxed{\frac{1}{R}\frac{d\delta}{dk} = \frac{\Delta t}{\left(\frac{2R}{v_0}\right)} = \frac{\text{delay}}{\text{free transit time}}\,.} \tag{1.22}$$

The left-hand side is unit free, and the right hand side is the ratio of the time delay to the time the free particle would take to travel in and out of the range R.

1.2 An Example

Consider the following example in which we have an attractive potential:

$$V(x) = \begin{cases} -V_0\,, & \text{for} \quad 0 < x < a\,, \\ 0\,, & \text{for} \quad x > a\,, \\ \infty\,, & \text{for} \quad x < 0\,. \end{cases} \tag{1.23}$$

The potential is shown in Figure 4 where the energy $E > 0$ of the energy eigenstate is indicated with a dashed line. The solution is of the form

$$\psi(x) = \begin{cases} e^{i\delta}\sin(kx+\delta) & x > a\,, \\ A\sin(k'x) & 0 < x < a\,. \end{cases} \tag{1.24}$$

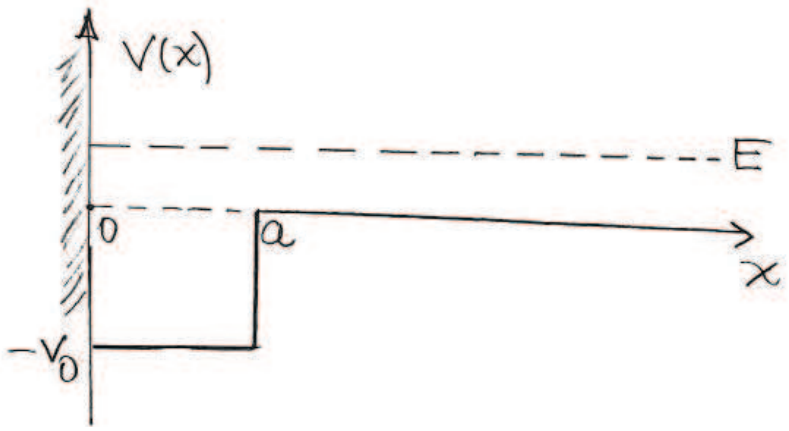

Figure 4: An attractive potential. We are interested in calculating the energy eigenstates for all $E > 0$.

The solution in the region $x > a$ is simply the canonical solution, and the solution in the region $x < a$ follows because we must have $\psi(0) = 0$. The constants k and k' are given by

$$k^2 \;=\; \frac{2mE}{\hbar^2}\,, \qquad k'^2 \;=\; \frac{2m(E+V_0)}{\hbar^2}\,. \tag{1.25}$$

Matching ψ and ψ' at $x = a$ we find the conditions that will eventually give us the unknown phase shift δ:

$$A\sin(k'a) = e^{i\delta}\sin(ka+\delta) \tag{1.26}$$

$$k'A\cos(k'a) = ke^{i\delta}\cos(ka+\delta). \tag{1.27}$$

Dividing the latter equation by the former, we reach

$$k\cot(ka+\delta) = k'\cot k'a. \tag{1.28}$$

We now make use of the identity

$$\cot(A+B) = \frac{\cot A\cot B - 1}{\cot A + \cot B}, \tag{1.29}$$

from which we find

$$\frac{k'}{k}\cot k'a = \cot(ka+\delta) = \frac{\cot ka\cot\delta - 1}{\cot ka + \cot\delta}. \tag{1.30}$$

Solving this equation for $\cot\delta$ yields

$$\boxed{\cot\delta = \frac{\tan ka + \frac{k'}{k}\cot k'a}{1 - \frac{k'}{k}\cot k'a\tan ka}.} \tag{1.31}$$

While this is a complicated formula to analyze directly, we can always plot it with a computer for different values of V_0. As usual we characterize the well by the constant z_0, defined by

$$z_0^2 \;=\; \frac{2mV_0a^2}{\hbar^2}\,. \tag{1.32}$$

Note also that

$$k'a \;=\; \sqrt{z_0^2 + (ka)^2}\,. \tag{1.33}$$

Figure 5 shows the phase factor δ, the quantity $\sin^2\delta$, the time delay $\frac{1}{a}\frac{d\delta}{dk}$, and the amplitude $|A|$ inside the well as functions of ka, for $z_0^2 = 3.40$.

Note that the phase δ begins at 0 for zero energy and reaches $-\pi$ for infinite energy. The excursion of the phase is thus π and as we will see, this happens because for this value of z_0 the potential would have one bound state.

The value of $|A_s|^2 = \sin^2\delta$ represents the probability of scattering and it peaks for the value of ka for which the phase δ has absolute value $\pi/2$.

Next in the plot is the unit-free delay $\frac{1}{a}\frac{d\delta}{dk}$. Notice that the delay is negative. This is easily explained: as the particle moves over the well, its kinetic energy is increased by V_0, the particle speeds up as it reaches and bounces off the wall.

The last plot shows the magnitude $|A|$ of the constant that gives the amplitude of the wavefunction in the region $0 < x < a$.

At very large energy $E \gg V_0$, the particle hardly notices the potential. Indeed we see that δ approaches $-\pi$ which, as noted below (1.8), is equivalent to $\delta = 0$ and means no phase shift. Accordingly $\sin^2\delta \to 0$, meaning no scattering. We also have $\frac{1}{a}\frac{d\delta}{dk} \to 0$, meaning no time delay and, finally, $|A| \to 1$ as in the free solution.

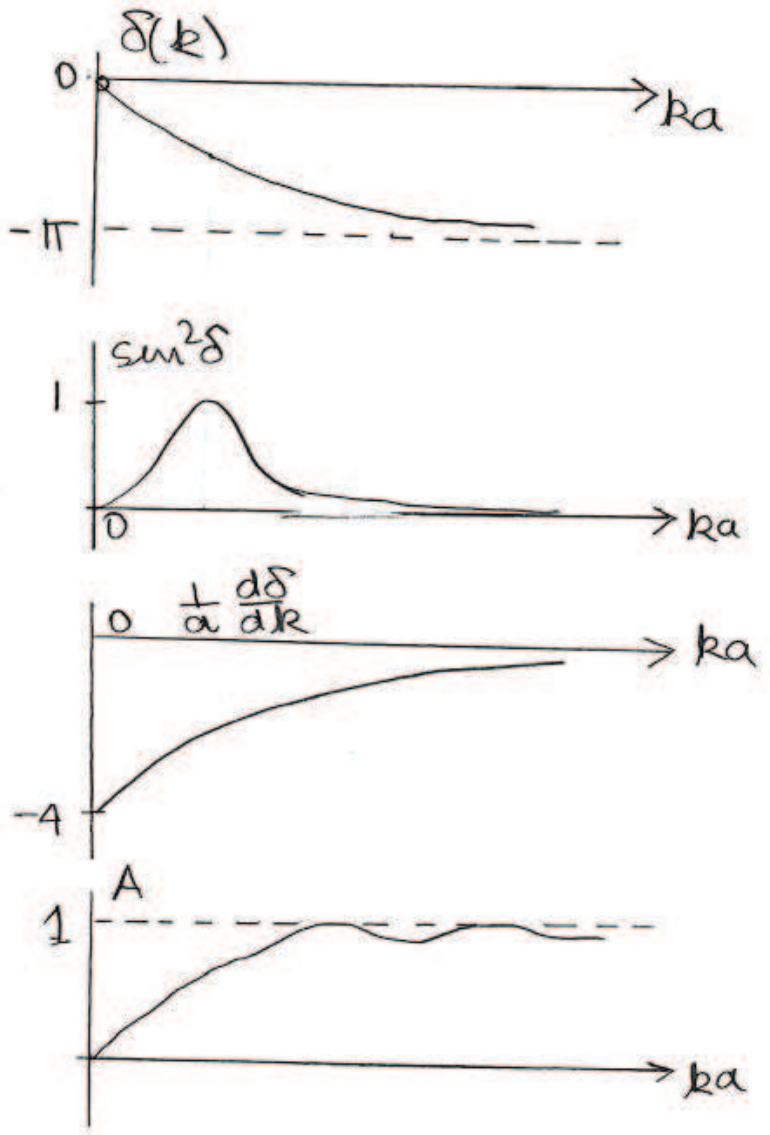

Figure 5: Various quantities plotted as functions of ka, for $z_0^2 = 3.40$. Top: the phase shift, going from zero to $-\pi$. Second: the scattering amplitude $|A_s|^2 = \sin^2\delta$. Third: the delay relative to the free transit time. Last: the norm $|A|$ of the amplitude of the wave inside the well.

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lecture 19

B. Zwiebach
April 28, 2016

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1 Levinson's Theorem

Levinson's theorem relates the number N_b of bound states of a given potential to the excursion of the phase shift $\delta(E)$ as the energy goes from zero to infinity:

$$\boxed{N_b \;=\; \frac{1}{\pi}(\delta(0)-\delta(\infty))\,.} \tag{1.1}$$

To prove this result consider an arbitrary potential $V(x)$ of range R, with a wall at $x = 0$. This potential, shown to the left in Figure 1, has a number of bound states, all of which are non-degenerate and can be counted. There is also a set of positive energy eigenstates: the scattering states that, belonging to a continuum, cannot be counted. Our proof requires the possibility of counting states, so we will introduce a second infinite wall, placed at $x = L$ for large L. Of course, this will change the spectrum, but as L becomes larger and larger the changes will become smaller and smaller. We think of L as a *regulator* for the potential that discretizes the spectrum and thus enables us to enumerate the states. It does so because with two walls, the potential becomes a wide infinite well and all states become bound states. The potential with the regulator wall is shown to the right in Figure 1.

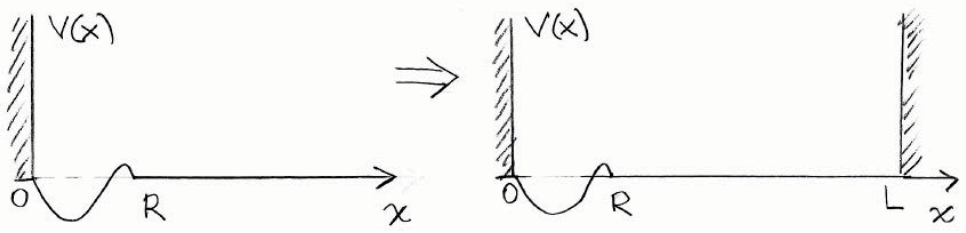

Figure 1: Left: An arbitrary one-dimensional potential $V(x)$ of range R. Right: The same potential with a regulator wall placed at $x = L$.

The key of the proof will be to compare the counting of states in the regulated $V \neq 0$ potential to the counting of states in the $V = 0$ potential, also regulated with a second wall at $x = L$. Consider therefore the regulated $V = 0$ potential and the *positive* energy eigenstates. These correspond to the wavefunction $\phi(x) = \sin kx$, with the second wall requiring $\phi(x = L) = 0$. We thus have

$$kL = n\pi, \quad \text{with} \quad n = 1, 2, \ldots \tag{1.2}$$

The values of k are now quantized. Let dk be an **infinitesimal** interval in wavenumber with dn the number of states in dk when $V = 0$. Thus,

$$dk\, L = dn\, \pi \quad \rightarrow \quad dn \;=\; \frac{L}{\pi}\, dk\,. \tag{1.3}$$

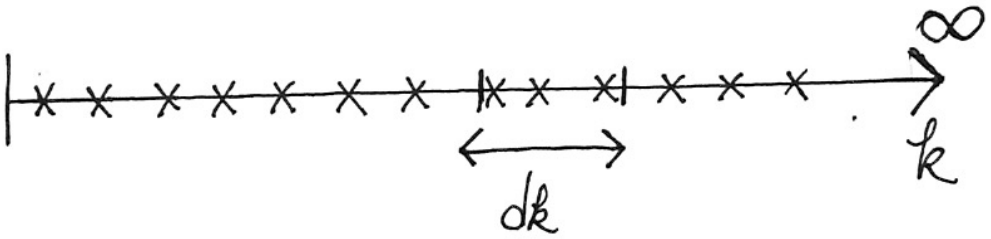

Figure 2: With the regulator wall the wavenumber k takes discrete values. dk is an **infinitesimal** interval in k space.

When $V(x) \neq 0$, the solutions for $x > R$, all of which are *positive* energy solutions, have the form

$$\psi(x) = e^{i\delta} \sin(kx + \delta)\,. \tag{1.4}$$

The boundary condition $\psi(L) = 0$ implies a quantization

$$kL + \delta(k) \;=\; n'\pi\,, \tag{1.5}$$

with n' integer. We can again differentiate to determine the number of positive energy states dn' in the interval dk, with $V \neq 0$:

$$dkL + \frac{d\delta}{dk}\, dk \;=\; dn'\pi \quad \rightarrow \quad dn' = \frac{L}{\pi} dk + \frac{1}{\pi}\left(\frac{d\delta}{dk}\right) dk\,. \tag{1.6}$$

The number of positive energy solutions *lost* in the interval dk as we turn on the potential V is given by $dn - dn'$, which can be evaluated using (1.3) and (1.6):

$$dn - dn' \;=\; -\frac{1}{\pi}\left(\frac{d\delta}{dk} dk\right). \tag{1.7}$$

The total number of positive energy solutions lost as the potential V is turned on is given by integrating the above over the full range of k:

$$\#\text{ of positive energy solutions lost as } V \text{ turns on } \;=\; -\int_0^\infty \frac{1}{\pi}\frac{d\delta}{dk} dk \;=\; -\frac{1}{\pi}(\delta(\infty) - \delta(0))\,. \tag{1.8}$$

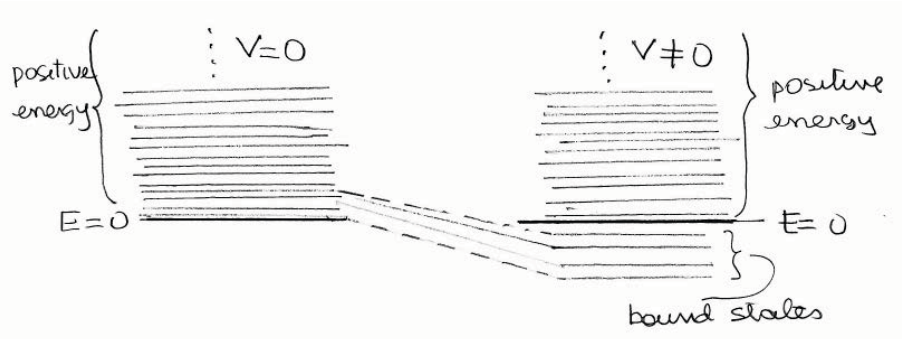

Figure 3: The positive energy states of the $V = 0$ setup shift as the potential is turned on and some can become bound states.

Although we lose a number of positive energy solutions as the potential V is turned on, states do not disappear. As one turns on the potential from zero to V continuously, we can track each energy eigenstate and no state can disappear! If we lose some positive energy states those states must now appear as negative energy states, or bound states! Letting N_b denote the number of bound states in the $V \neq 0$ potential, the result in (1.8) implies that

$$N_b \;=\; \frac{1}{\pi}(\delta(0) - \delta(\infty))\,. \tag{1.9}$$

This is what we wanted to prove!

2 Resonances

We have calculated the time delay $\Delta t = 2\hbar\delta'(E)$ associated with the **reflected** wavepacket that emerges from the range R potentials we have considered. If the time delay is negative, the **reflected** wavepacket emerges ahead of time. We can ask: Can we get an arbitrarily large *negative* time delay? The answer is no. A very large time delay would be a violation of causality. It would mean that the incoming packet is **reflected** even before it reaches $x = R$, which is impossible. In fact, the largest negative time delay would be realized (at least classically) if we had perfect **reflection** when the incoming packet hits $x = R$. If this happens, the time delay would be $-\frac{2R}{v_0}$, where v_0 is the velocity of the packet. Indeed, $\frac{2R}{v_0}$ is the time saved by the packet that did not have to go in and out the range. Thus we expect

$$\text{time delay} \;=\; 2\hbar\frac{d\delta}{dE} \geq -\frac{2R}{v_0}\,. \tag{2.1}$$

This can be **simplified** a bit by using k derivatives

$$2\hbar\frac{d\delta}{dE} \;=\; 2\hbar\frac{1}{\frac{dE}{dk}}\frac{d\delta}{dk} \;=\; \frac{2}{v_0}\frac{d\delta}{dk} \geq -\frac{2R}{v_0}\,, \tag{2.2}$$

which then gives the constraint

$$\frac{d\delta}{dk} \;\geq\; -R\,. \tag{2.3}$$

The argument was not rigorous but the result is rather accurate, receiving corrections that vanish for packets of large energy.

Alternatively, we can ask: Can we get an arbitrarily large *positive* time delay? The answer is yes. This can happen if the wave packet gets temporarily trapped in the potential. In that case we would expect the probability amplitude to become large in the $0 < x < R$ region. If the wavepacket is trapped for a long time we have a **resonance**. The state is a bit like a bound state in that it gets localized in the potential, at least for a while. In order to get a resonance it helps to have an attractive potential and a positive energy barrier. We can achieve that with the potential

$$V(x) \;=\; \begin{cases} \infty & \text{for} \quad x \leq 0 \\ -V_0 & \text{for} \quad 0 < x < a \\ V_1 & \text{for} \quad a < x < 2a \\ 0 & \text{for} \quad x > 2a\,. \end{cases} \tag{2.4}$$

The potential, with $V_0, V_1 > 0$, is shown in **figure** 4. In order to have a resonance we take explore energies in the range zero to V_1. In such range of energies we can expect to **find** some particular values

that lead to resonant behavior, namely, large time delay and large amplitude for the wavefunction in the well.

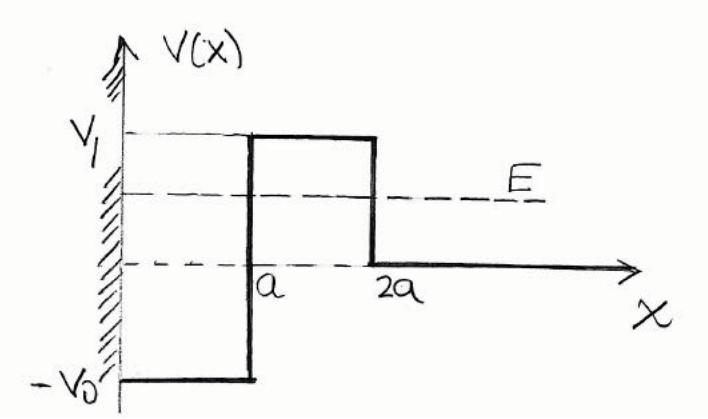

Figure 4: We search for resonances with energy E in the range $(0, V_1)$. In this range the V_1 barrier produces a classically forbidden region $x \in (a, 2a)$, that can help localize the amplitude around the well.

Given the three relevant regions in the potential we define

$$k'^2 = \frac{2m(E+V_0)}{\hbar^2}\,, \qquad \kappa^2 = \frac{2m(V_1-E)}{\hbar^2}\,, \qquad k^2 = \frac{2mE}{\hbar^2}\,. \tag{2.5}$$

In the region $0 < x < a$ we must use trigonometric functions of $k'x$. In the region $a < x < 2a$ we use hyperbolic functions of κa and in the region $x > 2a$ we use the canonical solution with phase shift and wavenumber k. In the middle region $a < x < 2a$ we could use a combination of solutions

$$\{e^{\kappa x},\ e^{-\kappa x}\}, \quad \text{or} \quad \{\cosh\kappa x\,,\ \sinh\kappa x\}\,, \quad \text{or} \quad \{\cosh\kappa(x-a)\,,\ \sinh\kappa(x-a)\}\,. \tag{2.6}$$

The last pair is most suitable to implement directly the continuity of the wavefunction at $x = a$. So we can write for the wavefunction $\psi(x)$:

$$\psi(x) = \begin{cases} A\sin(k'x) & 0 < x < a \\ A\sin(k'a)\cosh\kappa(x-a) \;+\; B\sinh\kappa(x-a) & a < x < 2a \\ e^{i\delta}\sin(kx+\delta) & x > 2a \end{cases} \tag{2.7}$$

After implementing the remaining boundary conditions we can solve for the phase shift δ. After a modest amount of work one finds:

$$\tan(2ka+\delta) = \frac{ka}{\kappa a}\cdot\frac{\sin k'a\,\cosh\kappa a \;+\; \frac{k'}{\kappa}\cos k'a\,\sinh\kappa a}{\sin k'a\,\sinh\kappa a \;+\; \frac{k'}{\kappa}\cos k'a\,\cosh\kappa a}\,. \tag{2.8}$$

This expression is fairly intricate so it is best to do numerical work. For this we define

$$z_0^2 \;=\; \frac{2mV_0a^2}{\hbar^2}\,, \quad z_1^2 \;=\; \frac{2mV_1a^2}{\hbar^2}\,, \quad u \;\equiv\; ka\,. \tag{2.9}$$

which allow us to express both $k'a$ and κa as functions of u

$$(k'a)^2 \;=\; z_0^2 + u^2\,, \quad (\kappa a)^2 \;=\; z_1^2 - u^2\,. \tag{2.10}$$

At this point (2.8) can be used to determine δ as a function of $u = ka$ and the constants z_0, z_1. Suppose we pick values for our parameter controlling equations. In Figure 5 we show results for $z_0^2 = 1$ and $z_1^2 = 5$.

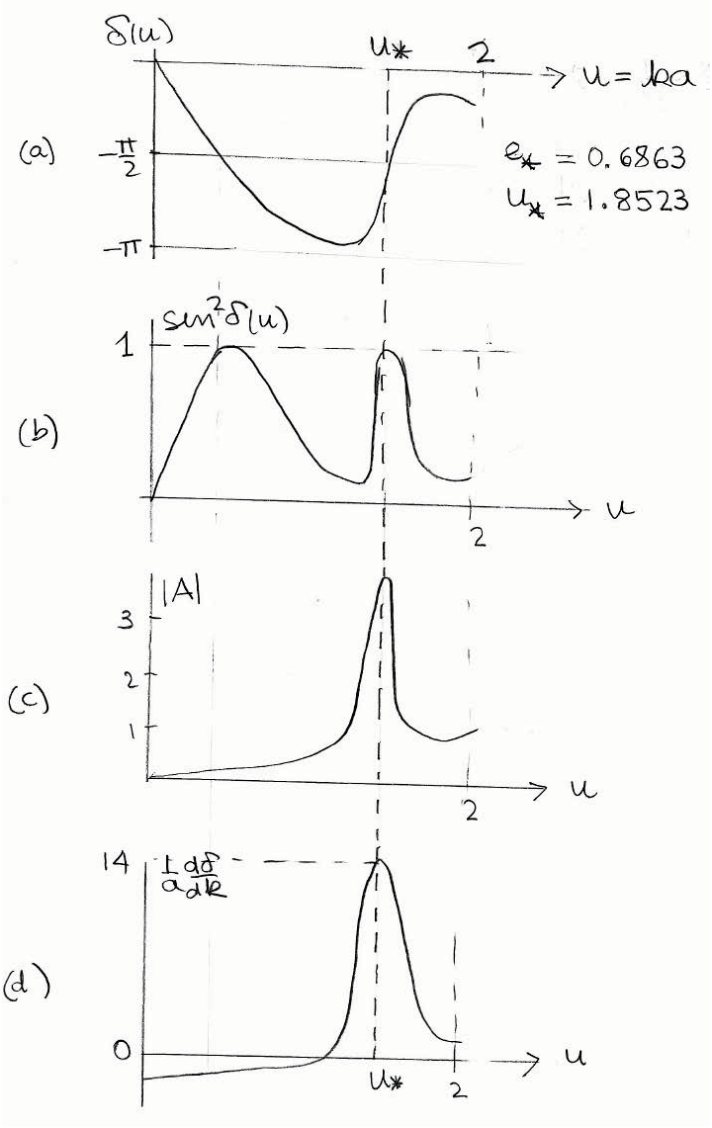

Figure 5: Plot of various quantities as a function of $u = ka$, with the potential characterized by $z_0^2 = 1$ and $z_0^2 = 5$. (a) $\delta(E)$ increases quickly around $u_* = 1.85$, or equivalently $E = 0.69V_1$, crossing $-\pi/2$ and signaling resonant behavior. (b) Plot of $|A_s|^2 = \sin^2\delta$, showing peaks each time $|\delta| = \pi/2$. (c) The coefficient $|A|$ of the wavefunction at the well peaks at the resonance, showing high probability of finding the particle at the well. (d) The time delay is positive and peaks at resonance.

Consider part (a) of the figure, showing $\delta(ka)$. At the beginning δ decreases linearly, a sign of a negative time delay, as the low energy waves reflect at the edge $x = 2a$ of the V_1 barrier. As δ crosses $-\pi/2$ there is no resonance, even though $|A_s|^2 = \sin^2\delta$ is equal to one. Indeed we see no bump in the amplitude $|A|$. As the energy is increased and $u = u_* = 1.8523$ we get a resonance. This time δ is increasing rapidly and δ crosses $-\pi/2$ again, making $|A_s|^2 = 1$. The signal of resonance is the very

high $|A|$ the peak in the time delay. This time delay reaches the value of about 14, meaning the delay is fourteen times the free transit time $4a/v_0$!

3 Modeling the Resonance

We would like to have further insight into the nature of resonances. In particular we want to appreciate the general features of the phenomenon. Additionally, so far we can identify resonances by looking at the behavior of δ but, can we find an equation that defines resonances?

As a first step, we model the behavior of a phase near resonance. Recalling that a resonance requires $|\delta|$ cross the value $\pi/2$ and that δ, physically, is the same as δ increased or decreased by multiples of π we can choose to have δ vary from nearly zero to nearly π. We can achieve this with the following simple function.

$$\delta = \tan^{-1}\left(\frac{\beta}{\alpha - k}\right), \qquad \text{with} \quad \beta > 0\,, \quad \alpha > 0\,. \tag{3.1}$$

here α and β are positive constants with the same units as k. To see what this function does, we first plot the argument of the arc tangent at the top of Figure 6. Note that the argument varies quickly in the region $(\alpha - \beta, \alpha + \beta)$. The variation of the associated phase δ is shown in the figure below. To have a sharp increase in the phase we must have small β compared to α.

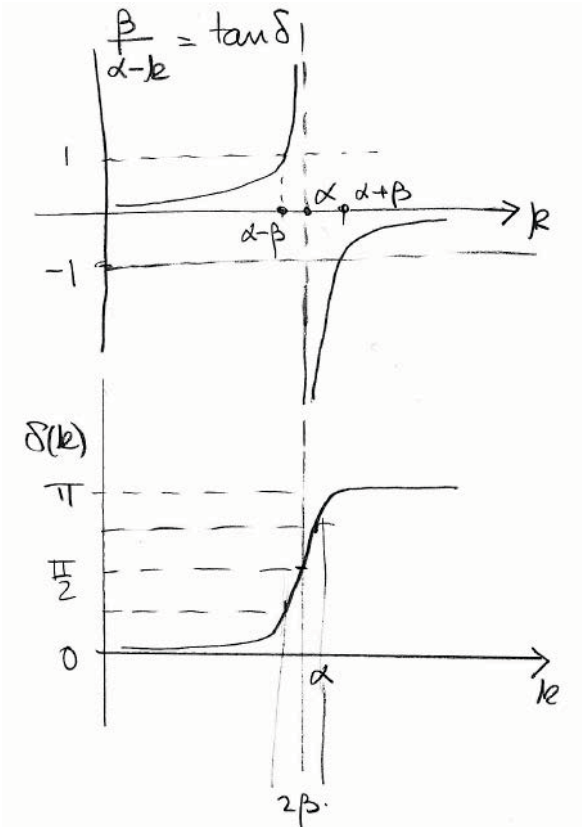

Figure 6: The constant β must be small compared to α to obtain a sharp variation. A resonance, as shown here requires δ increasing with energy.

Two relatively short calculations give us further insight:

$$\left.\frac{d\delta}{dk}\right|_{k=\alpha} = \frac{1}{\beta}, \quad |\psi_s|^2 = \sin^2\delta = \frac{\beta^2}{\beta^2+(\alpha-k)^2}. \tag{3.2}$$

The first one informs us that, all things being equal, the delay is large if β is small. The second gives the norm-squared of the scattering amplitude as a function of k, with a peak at $k=\alpha$. This equation is most famously expressed in terms of the energy. For this we note that

$$E - E_\alpha = \frac{\hbar^2}{2m}(k^2-\alpha^2) = \frac{\hbar^2}{2m}(k+\alpha)(k-\alpha) \simeq \frac{\hbar^2}{2m}(2\alpha)(k-\alpha), \tag{3.3}$$

when working with $k \approx \alpha$. It thus follows that

$$(k-\alpha)^2 \simeq \frac{m^2}{\hbar^4\alpha^2}(E-E_\alpha)^2, \tag{3.4}$$

and therefore

$$|\psi_s|^2 \simeq \frac{\beta^2}{\beta^2 + \frac{m^2}{\hbar^4\alpha^2}(E-E_\alpha)^2} = \frac{\frac{1}{4}\Gamma^2}{(E-E_\alpha)^2+\frac{1}{4}\Gamma^2}, \tag{3.5}$$

Where we have defined the constant Γ with units of energy:

$$\tfrac{1}{4}\Gamma^2 = \frac{\hbar^4\beta^2\alpha^2}{m^2} \quad \rightarrow \quad \Gamma = \frac{2\alpha\beta\hbar^2}{m}. \tag{3.6}$$

The energy dependence of $|\psi_s|^2$ follows the so-called *Breit-Wigner distribution*,

$$\boxed{|\psi_s|^2 \simeq \frac{\frac{1}{4}\Gamma^2}{(E-E_\alpha)^2+\frac{1}{4}\Gamma^2}.} \tag{3.7}$$

The distribution is shown in Figure 8. The peak value for $|\psi_s|^2$ is attained for $E=E_\alpha$ and is one. We call Γ the width at half-maximum because the value of $|\psi_s|^2$ at $E = E_\alpha \pm \frac{1}{2}\Gamma$ is one-half. Small Γ corresponds to a narrow width, or a narrow resonance.

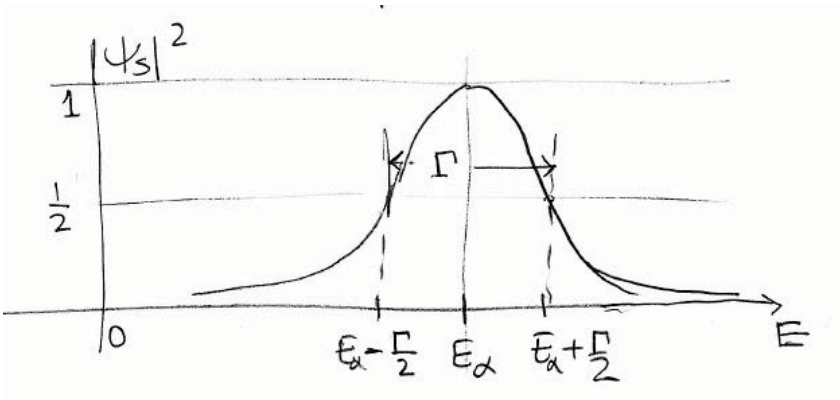

Figure 7: The Breit-Wigner distribution. Γ is the width of the distribution at half maximum.

To understand better the significance of Γ we define the associated time τ, called the **lifetime** of the resonance:

$$\tau \equiv \frac{\hbar}{\Gamma} = \frac{m}{2\alpha\beta\hbar}. \tag{3.8}$$

As you probably would expect, the lifetime is closely related to the time delay associated with a wavepacket of mean energy equal to the resonant energy. Indeed, we can evaluate the time delay Δt for $k = \alpha$ to get

$$\Delta t \;=\; 2\hbar \frac{d\delta}{dE} \;=\; 2\hbar \frac{dk}{dE}\,\frac{d\delta}{dk}\bigg|_{k=\alpha} = \frac{2\hbar}{\left(\frac{\hbar^2 k}{m}\right)}\left(\frac{1}{\beta}\right) = \frac{2\hbar}{\left(\frac{\hbar^2 \alpha\beta}{m}\right)} = \frac{2m}{\alpha\beta\hbar} = 4\tau\,. \tag{3.9}$$

We therefore conclude that the lifetime and the time delay are the same quantity, up to a factor of four.

$$\boxed{\;\tau \;=\; \frac{\hbar}{\Gamma} \;=\; \tfrac{1}{4}\,\Delta t\,.\;} \tag{3.10}$$

Unstable particles are sometimes called resonances. The Higgs boson, discovered in 2012, is an unstable particle with mass 125 GeV. It can decay into two photons, or into two **tau's**, or into a $b\bar{b}$ pair, among few possibilities. The width Γ associated to the particle is 4.07 Mev ($\pm 4\%$). Its lifetime τ is about 1.62×10^{-22} seconds!

We now try to understand resonances more mathematically. We saw that, at resonance, the norm of A_s reaches a maximum value of one. Let us explore when A_s is large. We have

$$A_s \;=\; \sin\delta\, e^{i\delta} \;=\; \frac{\sin\delta}{e^{i\delta}} \;=\; \frac{\sin\delta}{\cos\delta - i\sin\delta} \;=\; \frac{\tan\delta}{1 - i\,\tan\delta}\,. \tag{3.11}$$

At resonance $\delta = \pi/2$ and $A_s = i$, using the **first** equality. On the other hand, while we usually think of δ as a real number, the **final** expression above indicates that A_s becomes **infinite** for

$$\tan\delta \;=\; -i\,, \tag{3.12}$$

whatever that means! If we recall that $\tan iz = i\tanh z$ we deduce that the above condition requires $\delta \to -i\infty$, a rather strange result. At any rate, A_s becomes infinite, or has a pole, at $\tan\delta = -i$. We will see that the large value $|A_s| = 1$ at resonance can be viewed as the "**shadow**" of the **infinite** value A_s reaches nearby in the complex plane.

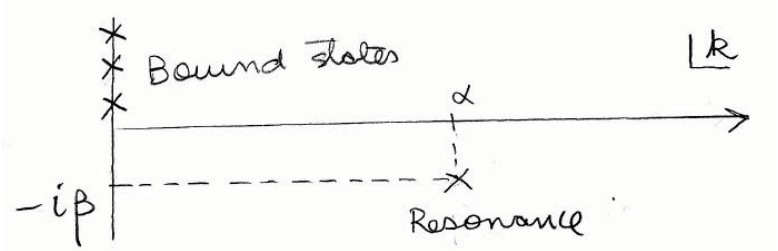

Figure 8: In the complex k plane, resonances are identified as poles of the scattering amplitude A_s located slightly below the real axis. Bound states appear as poles on positive imaginary axis.

Indeed, we can see how A_s behaves near resonance by inserting the near-resonance behavior (3.1) of δ into (3.11):

$$A_s \;=\; \frac{\frac{\beta}{\alpha - k}}{1 - i\frac{\beta}{\alpha - k}} \;=\; \frac{\beta}{(\alpha - i\beta) - k}\,. \tag{3.13}$$

When $k = \alpha$, meaning at the resonant energy, we get $A_s = i$, as expected. If we now think of the wavenumber k as a complex variable, we see that the pole of A_s is a pole at $k = k_* = \alpha - i\beta$. The real part of k_* is the resonant energy, and the imaginary part β encodes the lifetime. For small β the resonance is a pole near the real axis, as illustrated in Figure 8. The smaller β the sharper the resonance. As we can see, the value of $|A_s|$ on the real line becomes large for $k = \alpha$ because it is actually **infinite** a little below the axis.

The lesson in all of this is that we can indeed take (3.12) seriously and look for resonances by solving for the *complex* k values for which

$$\boxed{\text{Resonance condition:} \quad \tan\delta(k) \;=\; -i\,.} \tag{3.14}$$

The real part of those k's are the resonant energies. The imaginary parts give us the lifetime.

The idea of a complex k plane is very powerful. Suppose we consider purely imaginary k values of the form $k = i\kappa$, with $\kappa > 0$. Then the energy takes the form

$$E \;=\; -\frac{\hbar^2\kappa^2}{2m} < 0\,, \tag{3.15}$$

which is suitable for bound states. Indeed one can show that bound states appear as poles of A_s along the positive imaginary axis, as shown in Figure 8. The complex k-plane has room to **fit** scattering states, resonances, and bound states!

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lectures 20 and 21: Quantum Mechanics in 3D and Central Potentials

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1 Schrödinger Equation in 3D and Angular Momentum

We have so far considered a number of Hermitian operators: the position operator, the momentum operator, and the energy operator, or the Hamiltonian. These operators are observables and their eigenvalues are the possible results of measuring them on states. We will be discussing here another operator: angular momentum. It is a vector operator, just like momentum. It will lead to three components, each of which is a Hermitian operator, and thus a measurable quantity. The definition of the angular momentum operator, as you will see, arises from the classical mechanics counterpart. The properties of the operator, however, will be rather new and surprising.

You may have noticed that the momentum operator has something to do with translations. Indeed the momentum operator is a derivative in coordinate space and derivatives are related to translations. The precise way in which this happens is through exponentiation. Consider a suitable exponential of the momentum operator:

$$e^{\frac{i\hat{p}a}{\hbar}}\,, \tag{1.1}$$

where a is a constant with units of length, making the argument of the exponential unit free. Consider now letting this operator act on a wavefunction $\psi(x)$

$$e^{\frac{i\hat{p}a}{\hbar}}\psi(x) \;=\; e^{a\frac{d}{dx}}\psi(x)\,, \tag{1.2}$$

where we simplified the exponent. Expanding the exponential gives

$$\begin{aligned} e^{\frac{i\hat{p}a}{\hbar}}\psi(x) \;&=\; \Big(1 + a\frac{d}{dx} + \frac{a^2}{2!}\frac{d^2}{dx^2} + \frac{a^3}{3!}\frac{d^3}{dx^3} + \dots\Big)\psi(x)\,, \\ &=\; \psi(x) + a\frac{d\psi}{dx} + \frac{a^2}{2!}\frac{d^2\psi}{dx^2} + \frac{a^3}{3!}\frac{d^3\psi}{dx^3} + \dots \;=\; \psi(x+a)\,, \end{aligned} \tag{1.3}$$

since we recognize the familiar Taylor expansion. This result means that the operator $e^{\frac{i\hat{p}a}{\hbar}}$ moves the wavefunction. In fact it moves it a distance $-a$, since $\psi(x+a)$ is the displacement of $\psi(x)$ by a distance $-a$. We say that the momentum operator *generates* translations. Similarly, we will be able to show that the *angular momentum operator generates rotations*. Again, this means that suitable exponentials of the angular momentum operator acting on wavefunctions will rotate them in space.

Angular momentum can be of the orbital type, this is the familiar case that occurs when a particle rotates around some fixed point. But is can also be *spin* angular momentum. This is a rather different kind of angular momentum and can be carried by point particles. Much of the mathematics of angular momentum is valid both for orbital and spin angular momentum.

Let us begin our analysis of angular momentum by recalling that in three dimensions the usual $\hat{x}$ and $\hat{p}$ operators are vector operators:

$$\begin{aligned} \hat{\mathbf{p}} &= (\hat{p}_x, \hat{p}_y, \hat{p}_z) = \frac{\hbar}{i}\nabla = \frac{\hbar}{i}\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right). \\ \hat{\mathbf{x}} &= (\hat{x}, \hat{y}, \hat{z}). \end{aligned} \tag{1.4}$$

The commutation relations are as follows:

$$\begin{aligned} [\,\hat{x},\, \hat{p}_x\,] &= i\hbar, \\ [\,\hat{y},\, \hat{p}_y\,] &= i\hbar, \\ [\,\hat{z},\, \hat{p}_z\,] &= i\hbar. \end{aligned} \tag{1.5}$$

All other commutators are involving the three coordinates and the three momenta are zero!

Consider a particle represented by a three-dimensional wavefunction $\psi(x, y, z)$ moving in a three-dimensional potential $V(\mathbf{r})$. The Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{1.6}$$

We have a **central potential** if $V(\mathbf{r}) = V(r)$. A central potential has no angular dependence, the value of the potential depends only on the distance r from the origin. A central potential is spherically symmetric; the surfaces of constant potential are spheres centered at the origin and it is therefore rotationally invariant. The equation above for a central potential is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(r)\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{1.7}$$

This equation will be the main subject of our study. Note that the wavefunction is a full function of $\mathbf{r}$, it will only be rotational invariant for the simplest kinds of solutions. Given the rotational symmetry of the potential we are led to express the Schroödinger equation and energy eigenfunctions using spherical coordinates.

In spherical coordinates, the Laplacian is

$$\nabla^2\psi = (\nabla\cdot\nabla)\psi = \frac{1}{r}\frac{\partial^2}{\partial r^2}\big(r\psi\big) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\psi. \tag{1.8}$$

Therefore the Schrödinger equation for a particle in a central potential becomes

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}\,r + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\,\sin\theta\frac{\partial}{\partial\theta}\, + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]\psi + V(r)\psi = E\psi. \tag{1.9}$$

In our work that follows we will aim to establish two facts:

1. The angular dependent piece of the ∇^2 operator can be identified as the magnitude squared of the angular momentum operator

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \;=\; -\frac{\mathbf{L}^2}{\hbar^2} \tag{1.10}$$

where

$$\mathbf{L}^2=\hat{L}_x\hat{L}_x+\hat{L}_y\hat{L}_y+\hat{L}_z\hat{L}_z\,. \tag{1.11}$$

This will imply that the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}\,r-\frac{1}{r^2}\frac{\mathbf{L}^2}{\hbar^2}\right]\psi+V(r)\psi \;=\; E\psi \tag{1.12}$$

or expanding out

$$\boxed{-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}\,(r\psi)\;+\;\frac{\mathbf{L}^2}{2mr^2}\psi+V(r)\psi \;=\; E\psi\,.} \tag{1.13}$$

2. Eq. (1.7) is the relevant equation for the two-body problem when the potential satisfies

$$V(\mathbf{r}_1,\mathbf{r}_2)=V(|\mathbf{r}_1-\mathbf{r}_2|)\,, \tag{1.14}$$

namely, if the potential energy is just a function of the distance between the particles. This is true for the electrostatic potential energy between the proton and the electron forming a hydrogen atom. Therefore, we will be able to treat the hydrogen atom as a central potential problem.

2 The angular momentum operator

Classically, we are familiar with the angular momentum, defined as the cross product of $\mathbf{r}$ and $\mathbf{p}$: $\mathbf{L}=\mathbf{r}\times\mathbf{p}$. We therefore have

$$\begin{aligned}\mathbf{L}\;&=(L_x,L_y,L_z)\equiv\;\mathbf{r}\times\mathbf{p}\,,\\ L_x&=yp_z-zp_y\,,\\ L_y&=zp_x-xp_z\,,\\ L_z&=xp_y-yp_x\,.\end{aligned} \tag{2.1}$$

We use the above relations to define the quantum angular momentum operator $\hat{\mathbf{L}}$ and its components, the operators $(\hat{L}_x,\hat{L}_y,\hat{L}_z)$:

$$\begin{aligned}\hat{\mathbf{L}}\;&=(\hat{L}_x,\hat{L}_y,\hat{L}_z)\,,\\ \hat{L}_x&=\hat{y}\hat{p}_z-\hat{z}\hat{p}_y\,,\\ \hat{L}_y&=\hat{z}\hat{p}_x-\hat{x}\hat{p}_z\,,\\ \hat{L}_z&=\hat{x}\hat{p}_y-\hat{y}\hat{p}_x\,.\end{aligned} \tag{2.2}$$

In crafting this definition we saw no ordering ambiguities. Each angular momentum operator is the difference of two terms, each term consisting of a product of a coordinate and a momentum. But note that in all cases it is a coordinate and a momentum along different axes, so they commute. Had we written $\hat{L}_x=\hat{p}_z\hat{y}-\hat{p}_y\hat{z}$, it would have not mattered, it is the same as the $\hat{L}_x$ above. It is simple to

check that the angular momentum operators are Hermitian. Take $\hat{L}_x$, for example. Recalling that for any two operators $(AB)^\dagger = B^\dagger A^\dagger$ we have

$$(\hat{L}_x)^\dagger \;=\; (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)^\dagger \;=\; (\hat{y}\hat{p}_z)^\dagger - (\hat{z}\hat{p}_y)^\dagger \;=\; \hat{p}_z^\dagger \hat{y}^\dagger - \hat{p}_y^\dagger \hat{z}^\dagger \,. \tag{2.3}$$

Since all coordinates and momenta are Hermitian operators, we have

$$(\hat{L}_x)^\dagger \;=\; \hat{p}_z\hat{y} - \hat{p}_y\hat{z} \;=\; \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \;=\; \hat{L}_x \,, \tag{2.4}$$

where we moved the momenta to the right of the coordinates by virtue of vanishing commutators. The other two angular momentum operators are also Hermitian, so we have

$$\hat{L}_x^\dagger \;=\; \hat{L}_x \,, \quad \hat{L}_y^\dagger \;=\; \hat{L}_y \,, \quad \hat{L}_z^\dagger \;=\; \hat{L}_z \,. \tag{2.5}$$

All the angular momentum operators are observables.

Given a set of Hermitian operators, it is natural to ask what are their commutators. This computation enables us to see if we can measure them simultaneously. Let us compute the commutator of $\hat{L}_x$ with $\hat{L}_y$:

$$[\hat{L}_x, \hat{L}_y] \;=\; [\,\hat{y}\hat{p}_z - \hat{z}\hat{p}_y,\, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z\,] \tag{2.6}$$

We now see that these terms fail to commute only because $\hat{z}$ and $\hat{p}_z$ fail to commute. In fact the first term of $\hat{L}_x$ only fails to commute with the first term of $\hat{L}_y$. Similarly, the second term of $\hat{L}_x$ only fails to commute with the second term of $\hat{L}_y$. Therefore

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] \;&=\; [\,\hat{y}\hat{p}_z,\, \hat{z}\hat{p}_x\,] + [\hat{z}\hat{p}_y,\, \hat{x}\hat{p}_z\,] \\
&=\; [\,\hat{y}\hat{p}_z,\, \hat{z}]\hat{p}_x + \hat{x}[\hat{z}\hat{p}_y,\, \hat{p}_z\,] \\
&=\; \hat{y}\,[\,\hat{p}_z,\, \hat{z}]\,\hat{p}_x + \hat{x}\,[\hat{z},\, \hat{p}_z]\,\hat{p}_y \\
&=\; \hat{y}(-i\hbar)\hat{p}_x + \hat{x}(i\hbar)\hat{p}_y \\
&=\; i\hbar(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)\,.
\end{aligned} \tag{2.7}$$

We now recognize that the operator on the final right hand side is $\hat{L}_z$ and therefore,

$$[\,\hat{L}_x, \hat{L}_y\,] \;=\; i\hbar\,\hat{L}_z \,. \tag{2.8}$$

The basic commutation relations are completely cyclic, as illustrated in Figure 1. In any commutation relation we can cycle the position operators as in $\hat{x} \to \hat{y} \to \hat{z} \to \hat{x}$ and the momentum operators as in $\hat{p}_x \to \hat{p}_y \to \hat{p}_z \to \hat{p}_x$ and we will obtain another consistent commutation relation. You can also see that such cycling takes $\hat{L}_x \to \hat{L}_y \to \hat{L}_z \to \hat{L}_x$, by looking at (2.2). We therefore claim that we do not have to calculate additional angular momentum commutators, and (2.8) leads to

$$\boxed{\begin{aligned}
[\,\hat{L}_x, \hat{L}_y\,] \;&=\; i\hbar\,\hat{L}_z \,, \\
[\,\hat{L}_y, \hat{L}_z\,] \;&=\; i\hbar\,\hat{L}_x \,, \\
[\,\hat{L}_z, \hat{L}_x\,] \;&=\; i\hbar\,\hat{L}_y \,.
\end{aligned}} \tag{2.9}$$

This is the full set of commutators of angular momentum operators. The set is referred to as the **algebra of angular momentum**. Notice that while the operators $\hat{L}$ were defined in terms of coordinates and momenta, the final answer for the commutators do not involve coordinates nor momenta: commutators of angular momenta give angular momenta! The $\hat{L}$ operators are sometimes referred to

as *orbital* angular momentum, to distinguish them from spin angular momentum operators. The spin angular momentum operators $\hat{S}_x, \hat{S}_y$, and $\hat{S}_z$ cannot be written in terms of coordinates and momenta. They are more abstract entities, in fact their simplest representation is as two-by-two matrices! Still, being angular momenta they satisfy exactly the same algebra as their orbital cousins. We have

$$\begin{aligned} [\,\hat{S}_x, \hat{S}_y\,] &= i\hbar\,\hat{S}_z\,, \\ [\,\hat{S}_y, \hat{S}_z\,] &= i\hbar\,\hat{S}_x\,, \\ [\,\hat{S}_z, \hat{S}_x\,] &= i\hbar\,\hat{S}_y\,. \end{aligned} \tag{2.10}$$

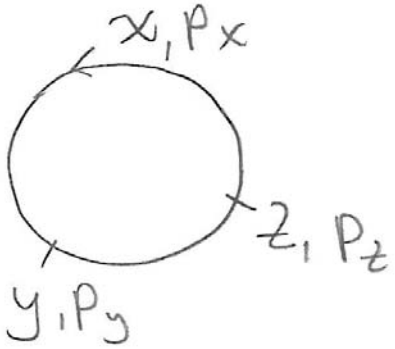

Figure 1: The commutation relations for angular momentum satisfy cyclicity).

We have seen that the commutator $[\hat{x}, \hat{p}] = i\hbar$ is associated with the fact that we cannot have simultaneous eigenstates of position and of momentum. Let us now see what the commutators of $\hat{L}$ operators tell us. In particular: can we have simultaneous eigenstates of $\hat{L}_x$ and $\hat{L}_y$? As it turns out, the answer is no, we cannot. We demonstrate this as follows. Let's assume that there exists a wavefunction ϕ_0 which is simultaneously an eigenstate of $\hat{L}_x$ and $\hat{L}_y$,

$$\begin{aligned} \hat{L}_x\,\phi_0 &= \lambda_x \phi_0\,, \\ \hat{L}_y\,\phi_0 &= \lambda_y \phi_0\,. \end{aligned} \tag{2.11}$$

Letting the first commutator identity of (2.9) act on ϕ_0 we have

$$\begin{aligned} i\hbar\hat{L}_z\phi_0 &= [\hat{L}_x, \hat{L}_y\,]\phi_0 = \hat{L}_x\hat{L}_y\phi_0 - \hat{L}_y\hat{L}_x\phi_0 \\ &= \hat{L}_x\lambda_y\phi_0 - \hat{L}_y\lambda_x\phi_0 \\ &= (\lambda_x\lambda_y - \lambda_y\lambda_x)\phi_0 = 0\,, \end{aligned} \tag{2.12}$$

showing that $\hat{L}_z\phi_0 = 0$. But this is not all, looking at the other commutators in the angular momentum algebra we see that they also vanish acting on ϕ_0 and as a result λ_x and λ_y must be zero:

$$\begin{aligned} \underbrace{[\,\hat{L}_y,\,\hat{L}_z\,]\phi_0}_{0} &= i\hbar\hat{L}_x\phi_0 = i\hbar\,\lambda_x\,\phi_0 \implies \lambda_x = 0\,, \\ \underbrace{[\,\hat{L}_z,\,\hat{L}_x\,]\phi_0}_{0} &= i\hbar\hat{L}_y\phi_0 = i\hbar\,\lambda_y\phi_0 \implies \lambda_y = 0\,. \end{aligned} \tag{2.13}$$

All in all, assuming that ϕ_0 is a simultaneous eigenstate of $\hat{L}_x$ and $\hat{L}_y$ has led to $\hat{L}_x\phi_0 = \hat{L}_y\phi_0 = \hat{L}_z\phi_0 = 0$. The state is annihilated by *all* angular momentum operators. This trivial situation is not

very interesting. We have learned that it is impossible to find states that are nontrivial simultaneous eigenstates of any two of the angular momentum operators.

For commuting Hermitian operators, there is no problem finding simultaneous eigenstates. In fact, commuting Hermitian operators always have a *complete* set of simultaneous eigenstates. Suppose we select $\hat{L}_z$ as one of the operators we want to measure. Can we now find a second Hermitian operator that commutes with it? The answer is yes. As it turns out, $\mathbf{L}^2$, defined in (1.11) commutes with $\hat{L}_z$ and is an interesting choice for a second operator. Indeed, we quickly check

$$\begin{aligned}
[\hat{L}_z, \hat{\mathbf{L}}^2] &= [\hat{L}_z, \hat{L}_x\hat{L}_x] + [\hat{L}_z, \hat{L}_y\hat{L}_y] \\
&= [\hat{L}_z, \hat{L}_x]\hat{L}_x + \hat{L}_x[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_y]\hat{L}_y + \hat{L}_y[\hat{L}_z, \hat{L}_y] \\
&= i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_x\hat{L}_y \\
&= 0\,.
\end{aligned} \tag{2.14}$$

So we should be able to find simultaneous eigenstates of both $\hat{L}_z$ and $\hat{L}^2$. We will do this shortly. The operator $\hat{\mathbf{L}}^2$ is **Casimir operator**, which means that it commutes with all angular momentum operators. Just like it commutes with $\hat{L}_z$, it commutes also with $\hat{L}_x$ and $\hat{L}_y$.

To understand the angular momentum operators a little better, let's write them in spherical coordinates. For this we need the relation between (r, θ, ϕ) and the cartesian coordinates (x, y, z):

$$\begin{aligned}
x &= r\sin\theta\cos\phi\,, & r &= \sqrt{x^2+y^2+z^2}\,, \\
y &= r\sin\theta\sin\phi\,, & \theta &= \cos^{-1}\!\big(\tfrac{z}{r}\big)\,, \\
z &= r\cos\theta\,, & \phi &= \tan^{-1}\!\big(\tfrac{y}{x}\big)\,.
\end{aligned} \tag{2.15}$$

We have hinted at the fact that angular momentum operators generate rotations. In spherical coordinates rotations about the z axis are the simplest: they change ϕ but leave θ invariant. Both rotations about the x and y axes change θ and ϕ. We can therefore hope that $\hat{L}_z$ is simple in spherical coordinates. Using the definition $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$ we have

$$\hat{L}_z \;=\; \frac{\hbar}{i}\Big(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\Big)\,. \tag{2.16}$$

Notice that this is related to $\frac{\partial}{\partial\phi}$ since, by the chain rule

$$\frac{\partial}{\partial\phi} \;=\; \frac{\partial y}{\partial\phi}\frac{\partial}{\partial y} + \frac{\partial x}{\partial\phi}\frac{\partial}{\partial x} + \cancelto{0}{\frac{\partial z}{\partial\phi}}\frac{\partial}{\partial z} \;=\; x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\,, \tag{2.17}$$

where we used (2.15) to evaluate the partial derivatives. Using the last two equations we can identify

$$\boxed{\hat{L}_z \;=\; \frac{\hbar}{i}\frac{\partial}{\partial\phi}\,.} \tag{2.18}$$

This is a very simple and useful representation. It confirms the interpretation that $\hat{L}_z$ generates rotations about the z axis, as it has to do with changes of ϕ. Note that $\hat{L}_z$ is like a momentum along the "circle" defined by the ϕ coordinate ($\phi = \phi + 2\pi$). The other angular momentum operators are a bit more complicated. A longer calculation shows what we suggested earlier, that

$$\boxed{-\frac{\hat{\mathbf{L}}^2}{\hbar^2} \;=\; \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,.} \tag{2.19}$$

3 Eigenstates of Angular Momentum

We demonstrated before that the Hermitian operators $\hat{L}_z$ and $\mathbf{L}^2$ commute. We now aim to construct the simultaneous eigenfunctions of these operators. They will be functions of θ and ϕ and we will call them $\psi_{\ell m}(\theta,\phi)$. The conditions that they be eigenfunctions are

$$\begin{aligned} \hat{L}_z\,\psi_{\ell m} &= \hbar m\,\psi_{\ell m}\,, & m &\in \mathbb{R} \\ \hat{\mathbf{L}}^2\,\psi_{\ell m} &= \hbar^2\,\ell(\ell+1)\,\psi_{\ell m}\,, & \ell &\in \mathbb{R}\,. \end{aligned} \tag{3.1}$$

As befits Hermitian operators, the eigenvalues are real. Both m and l are unit free; there is an $\hbar$ in the $\hat{L}_z$ eigenvalue because angular momentum has units of $\hbar$. For the eigenvalue of $\hat{\mathbf{L}}^2$ we have an $\hbar^2$. Note that we have written the eigenvalue of $\hat{\mathbf{L}}^2$ as $\ell(\ell+1)$ and for ℓ real this is always greater than or equal to $-1/4$. In fact $\ell(\ell+1)$ ranges from zero to infinity as ℓ ranges from zero to infinity. We can show that the eigenvalues of $\hat{\mathbf{L}}^2$ can't be negative. For this we first claim that

$$\big(\psi,\,\hat{\mathbf{L}}^2\psi\big) \geq 0\,, \tag{3.2}$$

and taking ψ to be a normalized eigenfunction with $\hat{\mathbf{L}}^2$ eigenvalue λ we immediately see that the above gives $\big(\psi,\,\lambda\psi\big) = \lambda \geq 0$, as desired. To prove the above equation we simply expand and use Hermiticity

$$\begin{aligned} \big(\psi,\,\hat{\mathbf{L}}^2\psi\big) &= \big(\psi,\,\hat{L}_x^2\psi\big) + \big(\psi,\,\hat{L}_x^2\psi\big) + \big(\psi,\,\hat{L}_x^2\psi\big) \\ &= \big(\hat{L}_x\psi,\,\hat{L}_x\psi\big) + \big(\hat{L}_y\psi,\,\hat{L}_y\psi\big) + \big(\hat{L}_z\psi,\,\hat{L}_z\psi\big) \geq 0\,, \end{aligned} \tag{3.3}$$

because each of the three summands is greater than or equal to zero.

Let us now solve the first eigenvalue equation in (3.1) using the coordinate representation (2.18) for the $\hat{L}_z$ operator:

$$\frac{\hbar}{i}\frac{\partial\psi_{\ell m}}{\partial\phi} = \hbar m\psi_{\ell m} \quad\to\quad \frac{\partial\psi_{\ell m}}{\partial\phi} = im\psi_{\ell m}\,. \tag{3.4}$$

This determines the ϕ dependence of the solution and we write

$$\psi_{\ell m}(\theta,\phi) = e^{im\phi}\,P_\ell^m(\theta)\,, \tag{3.5}$$

where the function $P_\ell^m(\theta)$ captures the still undetermined θ dependence of the eigenfunction $\psi_{\ell m}$. We will require that $\psi_{\ell m}$ be uniquely defined as a function of the angles and this requires that[1]

$$\psi_{\ell m}(\theta,\phi+2\pi) = \psi_{\ell m}(\theta,\phi)\,. \tag{3.6}$$

There is no similar condition for θ. The above condition requires that

$$e^{im(\phi+2\pi)} = e^{im\phi} \quad\to\quad e^{2\pi im} = 1\,. \tag{3.7}$$

This equation implies that m must be an integer:

$$\boxed{\,m \in \mathbb{Z}\,.} \tag{3.8}$$

[1] One may have tried to require that after ϕ increases by 2π the wavefunction changes sign, but this does not lead to a consistent set of $\psi_{\ell m}$'s.

This completes our analysis of the first eigenvalue equation. The second eigenvalue equation in (3.1), using our expression (2.19) for $\hat{\mathbf{L}}^2$, gives

$$-\hbar^2\Big(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big)\psi_{\ell m} \;=\; \hbar^2\ell(\ell+1)\psi_{\ell m}\,. \tag{3.9}$$

We multiply through by $\sin^2\theta$ and cancel the $\hbar^2$ to get

$$\Big(\sin\theta\frac{\partial}{\partial\theta}\,\sin\theta\frac{\partial}{\partial\theta}\,+\frac{\partial^2}{\partial\phi^2}\Big)\psi_{\ell m}=-\ell(\ell+1)\sin^2\theta\,\psi_{\ell m}\,. \tag{3.10}$$

Using $\psi_{\ell m}=e^{im\phi}P_\ell^m(\theta)$ we can evaluate the action of $\frac{\partial^2}{\partial\phi^2}$ on $\psi_{\ell m}$ and then cancel the overall $e^{im\phi}$ to arrive at the differential equation

$$\sin\theta\frac{d}{d\theta}\Big(\sin\theta\frac{dP_\ell^m}{d\theta}\Big)-m^2P_\ell^m=-\ell(\ell+1)P_\ell^m\sin^2\theta\,, \tag{3.11}$$

or, equivalently,

$$\sin\theta\frac{d}{d\theta}\Big(\sin\theta\frac{dP_\ell^m}{d\theta}\Big)+\big(\,\ell(\ell+1)\sin^2\theta-m^2\big)P_\ell^m \;=\; 0\,. \tag{3.12}$$

We now want to make it clear that we can view P_ℓ^m as a function of $\cos\theta$ by writing the differential equation in terms of $x=\cos\theta$. Indeed, this gives

$$\frac{d}{d\theta}=\frac{dx}{d\theta}\frac{d}{dx}=-\sin\theta\frac{d}{dx}\quad\to\quad\sin\theta\frac{d}{d\theta}\;=\;-(1-x^2)\frac{d}{dx}\,. \tag{3.13}$$

The differential equation becomes

$$(1-x^2)\frac{d}{dx}\Big[(1-x^2)\frac{dP_\ell^m}{dx}\Big]+\big[\ell(\ell+1)(1-x^2)-m^2\big]P_\ell^m(x)=0\,, \tag{3.14}$$

and dividing by $1-x^2$ we get the final form:

$$\boxed{\;\frac{d}{dx}\Big[(1-x^2)\frac{dP_\ell^m}{dx}\Big]+\Big[\ell(\ell+1)-\frac{m^2}{1-x^2}\Big]P_\ell^m(x)\;=\;0\,.\;} \tag{3.15}$$

The $P_\ell^m(x)$ are called the associated Legendre *functions*. They are not polynomials. All we know at this point is that m is an integer. We will discover soon that ℓ is a non-negative integer and that for a given value of ℓ there is a range of possible values of m.

To find out about ℓ we consider the above equation for $m=0$. In that case we write $P_\ell(x)\equiv P_\ell^0(x)$ and the $P_\ell(x)$ must satisfy

$$\frac{d}{dx}\Big[(1-x^2)\frac{dP_\ell}{dx}\Big]+\ell(\ell+1)P_\ell(x)\;=\;0\,. \tag{3.16}$$

This is the Legendre differential equation. We try finding a series solution by writing

$$P_\ell(x)=\sum_{k=0}^{\infty}a_kx^k\,, \tag{3.17}$$

assuming that $P_\ell(x)$ is regular at $x = 0$, as it better be. Plugging this into the DE yields we find that the vanishing of the coefficient of x^k requires:

$$(k+1)(k+2)a_{k+2} + [\ell(\ell+1) - k(k+1)]a_k \;=\; 0\,. \tag{3.18}$$

Equivalently, we have

$$\frac{a_{k+2}}{a_k} \;=\; -\,\frac{\ell(\ell+1) - k(k+1)}{(k+1)(k+2)}\,. \tag{3.19}$$

The large k behavior of the coefficients is such that unless the series terminates P_ℓ diverges at $x = \pm 1$ (since $x = \cos\theta$ this corresponds to $\theta = 0, \pi$). In order for the series to terminate, we must have $\ell(\ell+1) = k(k+1)$ for some integer $k \geq 0$. We can simply pick $\ell = k$ so that $a_{k+2} = 0$, making $P_k(x)$ a degree k polynomial. We have thus learned that the possible values of ℓ are

$$\boxed{\;\ell = 0, 1, 2, 3, \ldots\;} \tag{3.20}$$

This is quantization! Just like the m values are quantized, so are the ℓ values. The Legendre polynomials $P_\ell(x)$ are given by the Rodriguez formula:

$$P_\ell(x) \;=\; \frac{1}{2^\ell \ell!}\Big(\frac{d}{dx}\Big)^\ell \left(x^2 - 1\right)^\ell. \tag{3.21}$$

The Legendre polynomials have a nice generating function

$$\sum_{\ell=j}^{\infty} P_\ell(x) s^\ell = \frac{1}{\sqrt{1 - 2xs + s^2}}\;. \tag{3.22}$$

A few examples are

$$P_0(x) \;=\; 1\,, \quad P_1(x) \;=\; x\,, \quad P_2(x) \;=\; \tfrac{1}{2}\left(3x^2 - 1\right)\,. \tag{3.23}$$

$P_\ell(x)$ is a degree ℓ polynomial of definite parity.

Having solved the $m = 0$ equation we now have to discuss the general equation for $P_\ell^m(x)$. The differential equation involves m^2 and not m, so we can take the solutions for m and $-m$ to be the same. One can show that taking $|m|$ derivatives of the Legendre polynomials gives a solution for $P_\ell^m(x)$:

$$P_\ell^m(x) = (1 - x^2)^{|m|/2} \left(\frac{d}{dx}\right)^{|m|} P_\ell(x)\,. \tag{3.24}$$

Since P_ℓ is a polynomial of degree ℓ, the above gives a non-zero answer only for $|m| \leq \ell$. We thus have solutions for

$$\boxed{\;-\,\ell \leq m \leq \ell\,.\;} \tag{3.25}$$

It is possible to prove that no other solutions exist. One can think of the $\psi_{\ell m}$ eigenfunctions as first determined by the integer ℓ and, for a fixed ℓ, there are $2\ell + 1$ choices of m: $-\ell, -\ell + 1, \ldots, \ell$.

Our $\psi_{\ell m}$ eigenfunctions, with suitable normalization, are called the **spherical harmonics** $Y_{\ell m}(\theta, \phi)$. The properly normalized spherical harmonics for $m \geq 0$ are

$$Y_{\ell,m}(\theta, \phi) \;\equiv\; \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}(-1)^m e^{im\phi} P_\ell^m(\cos\theta). \tag{3.26}$$

For $m < 0$, we use

$$Y_{\ell,m}(\theta,\phi) = (-1)^m \left[Y_{\ell,-m}(\theta,\phi)\right]^* . \tag{3.27}$$

We thus have

$$\begin{aligned} \hat{L}_z\, Y_{\ell m} &= \hbar m\, Y_{\ell m}\,, \\ \hat{\mathbf{L}}^2\, Y_{\ell m} &= \hbar^2\, \ell(\ell+1)\, Y_{\ell m}\,. \end{aligned} \tag{3.28}$$

The first few spherical harmonics are

$$Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \tag{3.29}$$

$$Y_{1,\pm 1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}} e^{\pm i\phi} \sin\theta = \mp\sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r} \tag{3.30}$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos\theta = \sqrt{\frac{3}{4\pi}}\, \frac{z}{r^2}. \tag{3.31}$$

Being eigenstates of Hermitian operators with different eigenvalues, spherical harmonics with different ℓ and m subscripts are automatically orthogonal. The complicated normalization factor is needed to make them have unit normalization. The spherical harmonics form an orthonormal set with respect to integration over the solid angle. This integration can be written in many forms:

$$\int d\Omega\ \cdots = \int_0^{2\pi} d\phi \int_{\theta=0}^{\pi} d\theta\ \sin\theta \cdots = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\ \cdots . \tag{3.32}$$

The statement that the spherical harmonics form an orthonormal set with respect to this integration means that

$$\int d\Omega\ Y^*_{\ell',m'}(\theta,\phi) Y_{\ell,m}(\theta,\phi) = \delta_{\ell,\ell'}\delta_{m,m'}. \tag{3.33}$$

4 The Radial Wave Equation

Let us now write an ansatz for the solution of the Schrödinger equation. For this we take the product of a purely radial function $R_{E\ell}(r)$ and a spherical harmonic

$$\psi(r,\theta,\phi) = R_{E\ell}(r) Y_{\ell,m}(\theta,\phi). \tag{4.1}$$

We have put subscripts E and ℓ for the radial function. We did not include m, because, as we will see the equation for R does not depend on m. We can now insert this into the Schrödinger equation (1.13)

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r R_{E\ell} Y_{\ell m}\right) + \frac{\hat{\mathbf{L}}^2}{2mr^2} R_{E\ell} Y_{\ell m} + V(r) R_{E\ell} Y_{\ell m} = E R_{E\ell} Y_{\ell m}\,. \tag{4.2}$$

Since the spherical harmonics are $\hat{\mathbf{L}}^2$ eigenstates we can simplify the equation to give

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2(rR_{E\ell})}{dr^2}\, Y_{\ell m} + \frac{\hbar^2\ell(\ell+1)}{2mr^2} R_{E\ell} Y_{\ell m} + V(r) R_{E\ell} Y_{\ell m} = E R_{E\ell} Y_{\ell m}\,. \tag{4.3}$$

Canceling the common spherical harmonic and multiplying by r we get a purely radial equation

$$-\frac{\hbar^2}{2m}\frac{d^2(rR_{E\ell})}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2mr^2}(rR_{E\ell}) + V(r)(rR_{E\ell}) = E\,(rR_{E\ell})\,, \tag{4.4}$$

It is now convenient to define

$$u_{E\ell}(r) \;\equiv\; rR_{E\ell}(r)\,. \tag{4.5}$$

This allows us to rewrite the entire DE as

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2u_{E\ell}}{dr^2}+\Big(V(r)+\frac{\hbar^2\ell(\ell+1)}{2mr^2}\Big)u_{E\ell}=Eu_{E\ell}\,.} \tag{4.6}$$

This is called the **radial equation**. It looks like the familiar time-independent Schrödinger equation in one dimension, but with an effective potential

$$V_{\rm eff}(r) \;=\; V(r)+\frac{\hbar^2\ell(\ell+1)}{2mr^2}\,, \tag{4.7}$$

that features the original potential supplemented by a *centrifugal term*, a repulsive potential proportional to the angular momentum squared. Because of this term, the radial equation is slightly different for each value of ℓ. As anticipated, the quantum number m does not appear in the differential equation. The same radial solution $u_{E\ell}(r)$ must be used for all allowed values of m.

Recall our decomposition of the wavefunction:

$$\boxed{\psi(r,\theta,\phi) \;=\; R_{E\ell}(r)Y_{\ell,m}(\theta,\phi)=\frac{u_{E\ell}(r)}{r}Y_{\ell,m}(\theta,\phi)\,.} \tag{4.8}$$

The normalization condition requires

$$1=\int d^3x\;|\psi|^2=\int r^2drd\Omega\;\frac{|u_{E\ell}|^2}{r^2}Y^*_{\ell,m}Y_{\ell,m}\,. \tag{4.9}$$

The angular integral gives one, the explicit factors of r cancel and we get

$$\int_0^\infty dr\;|u_{E\ell}|^2=1. \tag{4.10}$$

Indeed $u_{E\ell}(r)$ plays the role of a one-dimensional wavefunction for a particle moving in the effective potential along r. Since only $r>0$ is allowed, we must consider the possible behavior of the wavefunction for $r=0$.

We can learn about the behavior of the radial solution at the origin under the reasonable assumption that the *centrifugal barrier dominates the potential as* $r\to 0$. In this case the most singular terms of the radial differential equation must cancel each other out, leaving less singular terms that we can ignore in this leading order calculation. So we set:

$$-\frac{\hbar^2}{2m}\frac{d^2u_{E\ell}}{dr^2}+\frac{\hbar^2\,\ell(\ell+1)}{2mr^2}u_{E\ell} \;=\; 0\,,\qquad \text{as } r\to 0\,. \tag{4.11}$$

or equivalently

$$\frac{d^2u_{E\ell}}{dr^2} \;=\; \frac{\ell(\ell+1)}{r^2}u_{E\ell}\,. \tag{4.12}$$

The solutions of this can be taken to be $u_{E\ell}=r^s$ with s a constant to be determined. We then find

$$s(s-1) \;=\; \ell(\ell+1) \quad\to\quad s=\ell+1,\; s=-\ell\,, \tag{4.13}$$

thus leading to two possible behaviors near $r = 0$:

$$u_{E\ell} \sim r^{\ell+1}, \quad \text{or} \quad u_{E\ell} \sim \frac{1}{r^{\ell}}. \tag{4.14}$$

For $\ell > 0$ the second behavior is not consistent with normalization, the wavefunction diverges at $r \to 0$ far too quickly. For $\ell = 0$ the second behavior, leading to $R \sim 1/r$, is in fact not a solution of the Schrödinger equation. Therefore we have established that for all $\ell \geq 0$ we must have

$$\boxed{u_{E\ell} \sim c\, r^{\ell+1}, \quad \text{as } r \to 0\,.} \tag{4.15}$$

Note that $u_{E\ell}$ vanishes at $r = 0$. Even for $\ell = 0$, we have $u \sim r$ and u vanishes at $r = 0$. Effectively there is an infinite wall at $r = 0$ consistent with the impossibility of extending r to negative values.

Recall that the full radial dependence of the wavefunction is obtained by dividing $u_{E\ell}$ by r, so that

$$R_{E\ell} \sim c\, r^{\ell}\,. \tag{4.16}$$

This allows for a constant non-zero wavefunction at the origin only for $\ell = 0$. Only for $\ell = 0$ a particle can be at the origin. For $\ell \neq 0$ the angular momentum "barrier" prevents the particle from reaching the origin.

Sarah Geller and Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

Lectures 21 and 22: Hydrogen Atom

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1 The Hydrogen Atom

Our goal here is to show that the two-body quantum mechanical problem of the hydrogen atom can be recast as one in which we have center-of-mass degrees of freedom that behave like a free particle and relative-motion degrees of freedom for which we have dynamics controlled by a central potential.

The hydrogen atom consists of a proton and an electron moving in three dimensions. We label the position and momentum operators of the proton as $\hat{\mathbf{x}}_p, \hat{\mathbf{p}}_p$, and those of the electron as $\hat{\mathbf{x}}_e, \hat{\mathbf{p}}_e$. These are canonical variables, meaning they satisfy the canonical commutation relations:

$$[(\hat{\mathbf{x}}_p)_i, (\hat{\mathbf{p}}_p)_j] = i\hbar\delta_{ij}, \quad [(\hat{\mathbf{x}}_e)_i, (\hat{\mathbf{p}}_e)_j] = i\hbar\delta_{ij}. \tag{1.1}$$

Here the subscripts $i, j = 1, 2, 3$ denote the various components of the vector operators. Furthermore, the proton variables **commute** with the electron variables. We have two pairs of *independent* canonical variables.

The wavefunction for the system is a function of the positions of both particles:

$$\Psi(\mathbf{x}_p, \mathbf{x}_e)\,, \tag{1.2}$$

and the quantity

$$|\Psi(\mathbf{x}_p, \mathbf{x}_e)|^2\, d^3\mathbf{x}_p\, d^3\mathbf{x}_e\,, \tag{1.3}$$

is the probability to find the proton within a window $d^3\mathbf{x}_p$ of $\mathbf{x}_p$ and the electron within a window $d^3\mathbf{x}_e$ of $\mathbf{x}_e$. The Hamiltonian of the system is given by

$$\hat{H} \;=\; \frac{\hat{\mathbf{p}}_p^2}{2m_p} + \frac{\hat{\mathbf{p}}_e^2}{2m_e} + V(|\mathbf{x}_e - \mathbf{x}_p|). \tag{1.4}$$

Note that the kinetic energy is simply the sum of the kinetic energy of the proton and kinetic energy of the electron. The potential only depends on the magnitude of the separation between the two particles, not on their individual positions.

In order to simplify the problem, we will introduce two new pairs of independent canonical variables. The first pair is associated with the center-of-mass (CM) motion. We introduce the total momentum operator $\hat{\mathbf{P}}$ and the CM position operator $\hat{\mathbf{X}}$, given by

$$\hat{\mathbf{P}} = \hat{\mathbf{p}}_p + \hat{\mathbf{p}}_e\,, \qquad \hat{\mathbf{X}} = \frac{m_e\hat{\mathbf{x}}_e + m_p\hat{\mathbf{x}}_p}{m_e + m_p}. \tag{1.5}$$

The operator $\hat{\mathbf{X}}$ is given by the typical expression for the center-of-mass of the system, but with the positions replaced by position operators. Using the commutation relations (1.1), we can show that $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$ are canonical conjugates:

$$\begin{aligned}\left[(\hat{\mathbf{X}})_i, (\hat{\mathbf{P}})_j\right] &= \left[\frac{m_e(\hat{\mathbf{x}}_e)_i + m_p(\hat{\mathbf{x}}_p)_i}{m_e+m_p}, (\hat{\mathbf{p}}_p)_j + (\hat{\mathbf{p}}_e)_j\right] \\ &= \frac{m_e}{m_e+m_p}\left[(\hat{\mathbf{x}}_e)_i\,, (\hat{\mathbf{p}}_e)_j\right] + \frac{m_p}{m_e+m_p}\left[(\hat{\mathbf{x}}_p)_i\,, \hat{\mathbf{p}}_p)_j\right] \\ &= \frac{m_e}{m_e+m_p}\, i\hbar\delta_{ij} + \frac{m_p}{m_e+m_p}\, i\hbar\delta_{ij}\,,\end{aligned} \tag{1.6}$$

resulting in the expected

$$\left[(\hat{\mathbf{X}})_i, (\hat{\mathbf{P}})_j\right] = i\hbar\delta_{ij}\,. \tag{1.7}$$

For the second pair of canonical variables we will define relative position and momentum operators. The relative position operator is the natural variable implied by the form of the potential:

$$\hat{\mathbf{x}} \;=\; \hat{\mathbf{x}}_e - \hat{\mathbf{x}}_p\,. \tag{1.8}$$

Since the second pair of canonical variables must commute with the first pair, we must check that $\mathbf{x}$ defined above, commutes with $\mathbf{X}$ and with $\mathbf{P}$. The commutation with $\mathbf{X}$ is automatic and the commutation with $\mathbf{P}$ works thanks to the minus sign in the above definition. We must now construct a relative momentum operator $\hat{\mathbf{p}}$ that is canonically conjugate to $\mathbf{x}$. It must be built from the momentum operators of the two particles, so we write

$$\hat{\mathbf{p}} = \alpha\,\hat{\mathbf{p}}_e - \beta\,\hat{\mathbf{p}}_p\,, \tag{1.9}$$

with α and β coefficients to be determined. To be canonically conjugate, the relative operators must satisfy

$$[(\hat{\mathbf{x}})_i, (\hat{\mathbf{p}})_j] = i\hbar\delta_{ij} \quad \rightarrow \quad \alpha+\beta \;=\; 1\,, \tag{1.10}$$

using the above definitions of $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$ and the proton and electron commutators. Finally, the relative momentum must commute with the CM coordinate

$$\left[(\hat{\mathbf{X}})_i, (\hat{\mathbf{p}})\right] = 0 \quad \rightarrow \quad m_e\alpha - m_p\beta = 0\,. \tag{1.11}$$

The two equations for α and β can be solved to find

$$\alpha = \frac{m_p}{m_e+m_p}, \quad \beta = \frac{m_e}{m_e+m_p}\,. \tag{1.12}$$

We define the total mass M and the reduced mass μ as follows

$$M = m_e + m_p, \quad \mu = \frac{m_e m_p}{m_e+m_p}\,. \tag{1.13}$$

The reduced mass of a pair of particles with very different masses is approximately equal to the mass of the lower-mass particle. Using these definitions

$$\alpha = \frac{\mu}{m_e}, \quad \beta = \frac{\mu}{m_p}. \tag{1.14}$$

Thus, collecting the relative variables we have

$$\hat{\mathbf{p}} \;=\; \mu\left(\frac{\hat{\mathbf{p}}_e}{m_e} - \frac{\hat{\mathbf{p}}_p}{m_p}\right) \;=\; \frac{m_p}{M}\,\hat{\mathbf{p}}_e - \frac{m_e}{M}\,\hat{\mathbf{p}}_p\,, \qquad \hat{\mathbf{x}} = \hat{\mathbf{x}}_e - \hat{\mathbf{x}}_p\,. \tag{1.15}$$

Note that the relative momentum $\mathbf{p}$ can be written in terms of velocities as follows: $\mathbf{p} = \mu(\mathbf{v}_e - \mathbf{v}_p)$. The relative momentum vanishes if the motion is only CM motion, in which case the velocities of the two parties are the same.

We can now rewrite the Hamiltonian in terms of the new variables. Solving for the original momentum operators in terms of $\hat{\mathbf{P}}$ and $\hat{\mathbf{p}}$, we find

$$\hat{\mathbf{p}}_p \;=\; \frac{m_p}{M}\,\hat{\mathbf{P}} - \hat{\mathbf{p}}, \qquad \hat{\mathbf{p}}_e \;=\; \frac{m_e}{M}\,\hat{\mathbf{P}} + \hat{\mathbf{p}}\,. \tag{1.16}$$

We can then rewrite the kinetic terms of the Hamiltonian in the form

$$\begin{aligned}\frac{\hat{\mathbf{p}}_p^2}{2m_p} + \frac{\hat{\mathbf{p}}_e^2}{2m_e} \;=\;& \frac{1}{2m_p}\left(\frac{m_p^2}{M^2}\hat{\mathbf{P}}^2 - \frac{2m_p}{M}\hat{\mathbf{P}}\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}^{\,2}\right) \\ &+ \frac{1}{2m_e}\left(\frac{m_e^2}{M^2}\hat{\mathbf{P}}^2 + \frac{2m_e}{M}\hat{\mathbf{P}}\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}^{\,2}\right) \\ &= \frac{\hat{\mathbf{P}}^2}{2M} + \frac{\hat{\mathbf{p}}^{\,2}}{2\mu}.\end{aligned} \tag{1.17}$$

Happily the term coupling the two momenta vanishes. Thus the center of mass degrees of freedom and the relative degrees of freedom give independent contributions to the kinetic energy. The Hamiltonian can then be written as

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2M} + \frac{\hat{\mathbf{p}}^{\,2}}{2\mu} + V(\,\hat{\mathbf{x}}\,). \tag{1.18}$$

In position space, the total and relative momentum operators can be expressed as gradients

$$\hat{\mathbf{P}} \;\to\; \frac{\hbar}{i}\nabla_{\mathbf{X}}, \qquad \hat{\mathbf{p}} \;\to\; \frac{\hbar}{i}\nabla_{\mathbf{x}}. \tag{1.19}$$

Each ∇ has a subscript indicating the type of coordinate we use to take the derivatives. Just like we had a wavefunction $\Psi(\mathbf{x}_e, \mathbf{x}_p)$ the new canonical variables require that we now think of the wavefunction as a function $\Psi(\mathbf{X}, \mathbf{x})$ of the new coordinates.

We solve the time-independent Schrödinger equation by using separation of variables

$$\Psi(\mathbf{X}, \mathbf{x}) = \Psi_{\rm CM}(\mathbf{X})\Psi_{\rm rel}(\mathbf{x}). \tag{1.20}$$

Plugging these into the time-independent Schrödinger equation $\hat{H}\Psi = E\Psi$, we reach

$$\left[\frac{\hat{\mathbf{P}}^2}{2M}\Psi_{\rm CM}(\mathbf{X})\right]\Psi_{\rm rel}(\mathbf{x}) + \left[\frac{\hat{\mathbf{p}}^{\,2}}{2\mu}\Psi_{\rm rel}(\mathbf{x}) + V(|\hat{\mathbf{x}}|)\Psi_{\rm rel}(\mathbf{x})\right]\Psi_{\rm CM}(\mathbf{X}) = E\Psi_{\rm CM}(\mathbf{X})\Psi_{\rm rel}(\mathbf{x}). \tag{1.21}$$

Dividing by the total wavefunction $\Psi_{\rm CM}(\mathbf{X})\Psi_{\rm rel}(\mathbf{x})$, this becomes

$$\frac{1}{\Psi_{\rm CM}(\mathbf{X})}\left[\frac{\hat{\mathbf{P}}^2}{2M}\Psi_{\rm CM}(\mathbf{X})\right] + \frac{1}{\Psi_{\rm rel}(\mathbf{x})}\left[\frac{\hat{\mathbf{p}}^{\,2}}{2\mu} + V(|\hat{\mathbf{x}}|)\right]\Psi_{\rm rel}(\mathbf{x}) = E. \tag{1.22}$$

The first term on the left-hand side is a function of $\mathbf{X}$ only and the second term on the left-hand side is a function of $\mathbf{x}$ only. Their sum is equal to the constant E and since $\mathbf{x}$ and $\mathbf{X}$ are independent variables, each term must individually be constant. We thus set the first term equal to the constant $E_{\rm CM}$ and the second term equal to the constant $E_{\rm rel}$, resulting in the following equations:

$$\frac{\hat{\mathbf{P}}^2}{2M}\Psi_{\rm CM}(\mathbf{X}) \;=\; E_{\rm CM}\Psi_{\rm CM}(\mathbf{X})\,, \tag{1.23}$$

$$\left[\frac{\hat{\mathbf{p}}^{\,2}}{2\mu} + V(|\mathbf{x}|)\right]\Psi_{\rm rel}(\mathbf{x}) \;=\; E_{\rm rel}\Psi_{\rm rel}(\mathbf{x})\,, \tag{1.24}$$

$$E = E_{\rm CM} + E_{\rm rel}. \tag{1.25}$$

We get two Schrödinger equations. The first equation tells us that the center of mass moves as a free particle of mass M. Thus, the CM energy is not quantized and we get plane wave solutions. The second equation is for the relative motion, and as we wanted to show, it is described as motion in a central potential. The third equation tells us that the total energy is the sum of the center-of-mass energy and the energy from the relative motion.

2 Hydrogen atom spectrum

We now have the tools to study the hydrogen atom, which has a central potential given by

$$V(r) \;=\; -\frac{Ze^2}{r}\,, \tag{2.1}$$

where Z is the number of protons in the nucleus. For hydrogen we have $Z = 1$. But it is worth considering $Z > 1$ in which case we are describing the motion of an electron around the nucleus of some other atom. We will also define following physical constants.

- The fine structure constant α: $\quad \alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}$.
- The *Bohr radius* a_0. This is the characteristic length scale in the problem. It can be calculated by equating kinetic and potential energies expressed in terms of a_0 and ignoring all numerical constants:

  $$\frac{\hbar^2}{m_e a_0^2} \;=\; \frac{e^2}{a_0}\,. \tag{2.2}$$

  Here the mass should be the reduced mass, which in this case can be taken rather accurately to be the mass of the electron. We then have explicitly,

  $$\begin{aligned} a_0 = \frac{\hbar^2}{me^2} = \frac{\hbar^2c^2}{e^2mc^2} = \frac{\hbar c}{\left(\frac{e^2}{\hbar c}\right)mc^2} = \frac{\hbar c}{\alpha mc^2} \\ = \frac{197\,\text{MeV fm}}{0.51\times10^6\,\text{eV}\left(\frac{1}{137}\right)} = \frac{1970\,\text{eV Angstrom}}{0.51\times10^6\,\text{eV}}\times 137 \\ = 0.529\,\text{Angstroms} \;\simeq 53\,\text{pm}. \end{aligned} \tag{2.3}$$

For the energy scale estimate we have

$$\frac{e^2}{a_0} = e^2\left(\frac{me^2}{\hbar^2}\right) = \left(\frac{e^4}{\hbar^2c^2}\right)mc^2 = \alpha^2mc^2 = \frac{1}{(137)^2}\times(511\,000\,\text{eV}) \;\simeq\; 27.2\ \text{eV} \tag{2.4}$$

There are other characteristic lengths that are interesting:

$$\begin{aligned} \alpha a_0 &= \text{Compton wavelength of electron} = \lambda_e \simeq 390\,\text{fm}\,, \\ \alpha^2 a_0 &= \text{classical electron radius} \simeq 2.8\,\text{fm}\,. \end{aligned} \tag{2.5}$$

Let us do some work now! The radial Schrödinger equation for bound states $E < 0$ reads

$$\Big(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} - \frac{Ze^2}{r}\Big) u = E\,u\,. \tag{2.6}$$

We could label the wavefunction u as $u_{E\ell}$ as the solutions will certainly depend on ℓ and the energy E. As usual, we like to work with a unit free coordinate. This could be achieved by writing $r = a_0 x$, with x unit free and a_0 carrying the length units of r. It will be more convenient to use a slight variation to eliminate Z from the equation and some factors of two. We will take the new unit-free coordinate x to be defined from

$$\boxed{\; r \equiv \frac{a_0}{2Z}\,x\,. \;} \tag{2.7}$$

The Schrödinger equation then becomes

$$\begin{aligned} &\Big(-\frac{\hbar^2}{2m}\frac{4Z^2}{a_0^2}\frac{d^2}{dx^2} + \frac{4Z^2}{a_0^2}\frac{\hbar^2}{2m}\frac{l(l+1)}{x^2} - \frac{2Z^2e^2}{a_0}\frac{1}{x}\Big) u = Eu \\ \to &\Big(\frac{2\hbar^2 Z^2}{ma_0^2}\Big(-\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2}\Big) - \frac{2Z^2e^2}{a_0}\frac{1}{x}\Big) u = Eu\,. \end{aligned} \tag{2.8}$$

Note that

$$\frac{2\hbar^2 Z^2}{ma_0^2} = \frac{2\hbar^2 Z}{ma_0}\frac{me^2}{\hbar^2} = \frac{2Ze^2}{a_0}\,, \tag{2.9}$$

which reduces our differential equation to

$$\Big(-\frac{d^2}{dx^2} + \frac{\ell(\ell+1)}{x^2} - \frac{1}{x}\Big) u = \frac{E}{\big(\frac{2Ze^2}{a_0}\big)}\,u\,. \tag{2.10}$$

We now define the unit-free parameter κ that encodes the energy:

$$\boxed{\; \kappa^2 = -\frac{E}{\big(\frac{2Ze^2}{a_0}\big)} > 0\,. \;} \tag{2.11}$$

κ is a unit-free version of the bound state energy. The differential equation is then

$$\boxed{\; \Big(-\frac{d^2}{dx^2} + \frac{\ell(\ell+1)}{x^2} - \frac{1}{x}\Big) u = -\kappa^2 u\,. \;} \tag{2.12}$$

We can further simplify this equation prior to solving it by examining the limiting cases. In the limit $x \to \infty$, the dominant terms are the second derivative and the term on the right-hand side, giving

$$\frac{d^2u}{dx^2} = \kappa^2 u \implies u \sim e^{\pm\kappa x}\,. \tag{2.13}$$

Since κ is unit free, we can make the above exponent equal to a new unit-free coordinate ρ:

$$\boxed{\rho \;\equiv\; \kappa\, x \;=\; \frac{2\kappa Z}{a_0}\, r\,.} \tag{2.14}$$

This time we get

$$\boxed{\Big(-\frac{d^2}{d\rho^2}+\frac{\ell(\ell+1)}{\rho^2}-\frac{1}{\kappa\,\rho}\Big)u \;=\; -u\,.} \tag{2.15}$$

Note that we did not get κ to disappear from the equation. This is good news: the equation should fix the possible values of κ (or possible energies). The equation above is not quite ready for a series solution: we would find a three term recursion relation, which is rather complicated. To make progress we discuss the behavior for small and large ρ.

For $\rho \to \infty$ we now get $u \sim u^{\pm\rho}$ and of course we hope for $u = e^{-\rho}$ for normalizability. As we discussed before, for $\rho \to 0$ the radial solution must be of the form $u \sim \rho^{(l+1)}$. This information about the behavior for small and for large ρ suggests a good ansatz for $u(\rho)$

$$\boxed{u(\rho) \;=\; \rho^{\ell+1}\, W(\rho)\, e^{-\rho}\,.} \tag{2.16}$$

where $W(\rho)$ is a yet to be determined function that we hope satisfies a simpler differential equation. To derive this differential equation for $W(\rho)$, we plug our ansatz into Eq. (2.15). As a little help on the calculation, we give an intermediate result:

$$-u''+\frac{\ell(\ell+1)}{\rho^2}u+u \;=\; \Big(-W''-\frac{2(\ell+1)}{\rho}W'+\frac{2(\ell+1)}{\rho}W+2W'\Big)\rho^{\ell+1}e^{-\rho}\,. \tag{2.17}$$

With a little more work we finally get the differential equation for W:

$$\boxed{\rho\frac{d^2W}{d\rho^2}+2(\ell+1-\rho)\frac{dW}{d\rho}+\Big[\frac{1}{\kappa}-2(\ell+1)\Big]\,W \;=\; 0\,.} \tag{2.18}$$

This looks a bit more complicated than the differential equation we started with but it leads to a very nice one-step recursion relation. As usual we write W as a series expansion

$$W=\sum_{k=0}^{\infty} a_k\rho^k\,, \tag{2.19}$$

and plugging back into (2.18), we group terms of order ρ^k to derive a recursion relation

$$\begin{aligned} & a_{k+1}k(k+1)+2(\ell+1)(k+1)a_{k+1}-2ka_k+\Big[\frac{1}{\kappa}-2(\ell+1)\Big]a_k \;=\; 0\,, \\ \to\quad & a_{k+1}(k(k+1)+2(\ell+1)(k+1)) \;=\; a_k\Big(2(\ell+k+1)-\frac{1}{\kappa}\Big)\,, \end{aligned} \tag{2.20}$$

which gives

$$\frac{a_{k+1}}{a_k} \;=\; \frac{2(k+\ell+1)-\frac{1}{\kappa}}{(k+1)(k+2\ell+2)}\,. \tag{2.21}$$

Detailed examination shows that for normalizable wave functions, the series must terminate. To see this we examine the large k behavior of the above ratio:

$$\frac{a_{k+1}}{a_k} \simeq \frac{2k}{k^2} = \frac{2}{k}\,. \tag{2.22}$$

Note that $\frac{2}{k+1} < \frac{2}{k}$; thus if the ratio $\frac{2}{k+1}$ leads to a divergence so will the ratio $\frac{2}{k}$. Taking

$$\frac{a_{k+1}}{a_k} = \frac{2}{k+1} \quad \to \quad a_{k+1} = \frac{2}{k+1} a_k\,, \tag{2.23}$$

and this is solved by

$$a_k = \frac{2^k}{k!}\, a_0\,. \tag{2.24}$$

Therefore, the sum

$$W = \sum_{k=0}^{\infty} a_k \rho^k \simeq a_0 \sum_{k=0}^{\infty} \frac{2^k \rho^k}{k!} = a_0 e^{2\rho}\,. \tag{2.25}$$

This is precisely sufficient to make the ansatz in (2.16) un-normalizable.

In order to get a normalizable solution the series for W must terminate. Suppose W is a polynomial of degree N so the coefficients satisfy

$$a_N \neq 0 \quad \text{and} \quad a_{N+1} = 0\,. \tag{2.26}$$

From Eq.(2.21) this implies

$$\frac{1}{\kappa} = 2(N + \ell + 1)\,. \tag{2.27}$$

Quantization has happened! The energy-encoding parameter κ is now related to integers! Note that ℓ can take values $\ell = 0, 1, 2, \ldots$ as it befits it being an angular momentum quantum number. Moreover N can take values $N = 0, 1, 2, \ldots$, since a polynomial of degree zero exists, being equal to a constant. Define the **principal** quantum number n as follows:

$$\boxed{n \equiv N + \ell + 1 = \frac{1}{2\kappa}\,, \quad \text{with } \ell = 0, 1, 2, \ldots\,,\ N = 0, 1, 2, \ldots\,, \text{ and } n = 1, 2, 3, \ldots\,.} \tag{2.28}$$

Importantly, note that for a fixed n we must have

$$0 \leq \ell \leq n - 1\,, \quad \text{and} \quad 0 \leq N \leq n - 1\,. \tag{2.29}$$

If n and ℓ are known, N is determined from $N + \ell + 1 = n$. So the independent quantum numbers so far are n and ℓ. Interestingly, the energies depend only on n, since κ depends only on n. Using Eq. (2.11), the energy dependence on principle quantum number is given by

$$E = -\frac{2Z^2 e^2}{a_0} \kappa^2\,, \tag{2.30}$$

and using $\kappa = \frac{1}{2n}$ we get

$$\boxed{E = -\frac{Z^2 e^2}{2a_0} \frac{1}{n^2}\,.} \tag{2.31}$$

These are the energy levels of the hydrogen atom! Since at any fixed value of $n > 1$ there are various possible ℓ values, the spectrum is highly degenerate. Even more, each value of ℓ amounts to $2\ell + 1$ states, given the possible values of m. One way to visualize the spectrum is shown in Figure 1. All integer points in the (N, ℓ) positive quadrant represent states. The states with common value of n lie on the dashed lines.

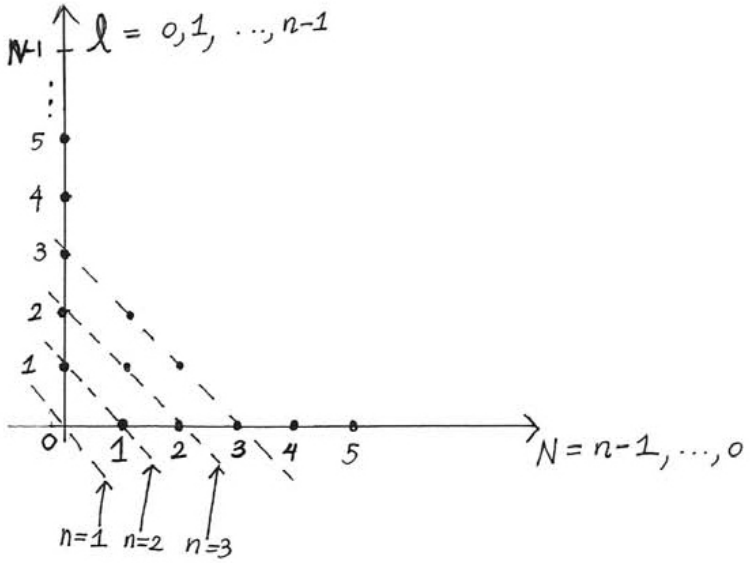

Figure 1: All points with integer $N \geq 0$ and integer $\ell \geq 0$ represent hydrogen atom states. The figure helps us to count the number of possible states for given value of n. Each dot along the diagonal line for a given n represents a possible state.

Figure 1 helps us to count the number of bound states for a given value of n. Recall that for each n, ℓ can take values from $0, ..., n-1$ and for each value of ℓ, m takes values from $-\ell$ to ℓ. The following table counts the states for the first few values of the principal quantum number n. A given state is specified by its values for (n, l, m), all of which are referred to as the *quantum numbers* for hydrogen states. Each number has a very important physical meaning: n tells us about the energy eigenvalue, $\hbar^2\ell(\ell+1)$ is the eigenvalue of the square of angular momentum and $\hbar m$ is the eigenvalue of the z component of angular momentum.

Number of States

n value	ℓ values	m values	total states
n=1	ℓ=0	m=0	1 state
n=2	ℓ=0	$m = 0$	1
	ℓ=1	$m = -1, 0, 1$	+ 3
			= 4 states
n=3	ℓ=0	$m = 0$	1
	ℓ=1	$m = -1, 0, 1$	+3
	ℓ=2	$m = -2, ..., 2$	+5
			= 9 states

The total number of states for arbitrary principal quantum number n can now be calculated:

$$\#\text{ of states for } n \;=\sum_{\ell=0}^{n-1}(2\ell+1) \;=\; \frac{2(n-1)n}{2} + n = n^2 - n + n = n^2\,. \tag{2.32}$$

This is in agreement with the partial results in the table. A more familiar representation of the states of hydrogen is given in Figure 2. The different columns indicate the different values of ℓ. We have also indicated in the figure the values of N, the degree of the polynomial entering the radial solution. Note that for a given ℓ, that is, for a fixed radial equation, the value of N increases as we go up the column. The number N corresponds to the number of nodes in the solution.

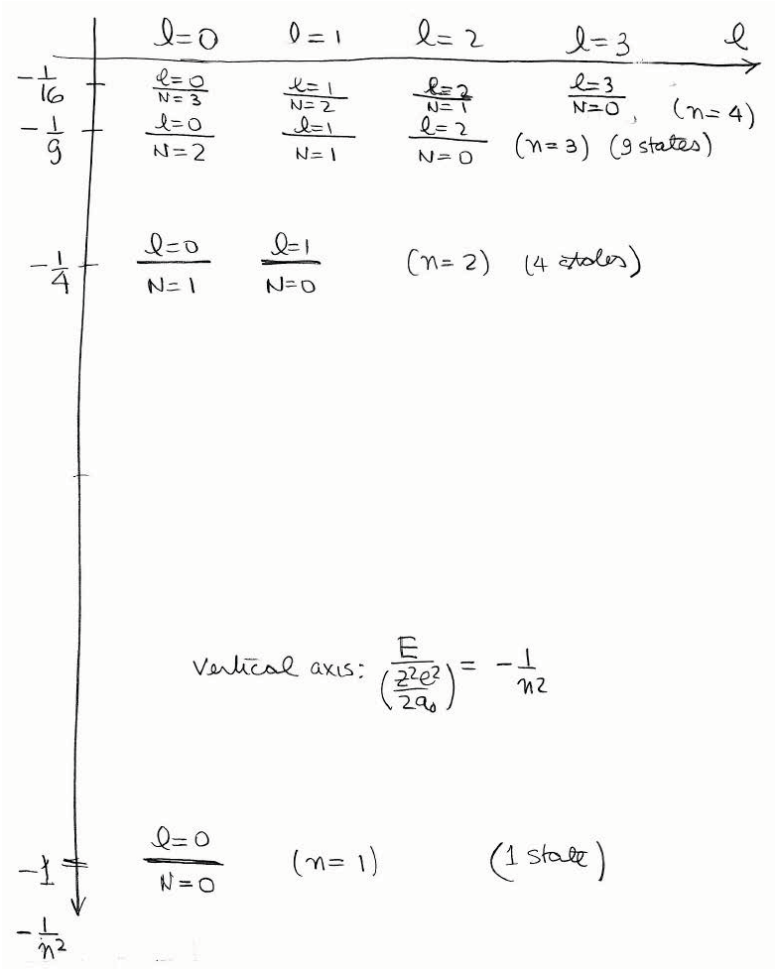

Figure 2: Plot of energy levels $E \sim -1/n^2$ indicating also the angular quantum number ℓ and the degree N of the polynomial. The spectrum is highly degenerate.

Recall that we defined $\rho = \frac{2\kappa Z r}{a_0}$. Together with $\kappa = \frac{1}{2n}$ this gives

$$\boxed{\rho = \frac{Zr}{na_0}\,.} \tag{2.33}$$

The eigenstates are labelled by quantum numbers (n, ℓ, m) and the wavefunctions are

$$\begin{aligned} \psi_{n\ell m} &= \mathcal{N}\, \frac{u_{n\ell}(r)}{r}\, Y_{\ell m}(\theta,\phi) \;=\; \mathcal{N}\, \frac{\rho^{\ell+1}}{\rho} W_{n\ell}(\rho) e^{-\rho}\, Y_{\ell m}(\theta,\phi) \\ &= \mathcal{N}\, \rho^{\ell} \underbrace{W_{n\ell}(\rho)}_{\substack{\text{polynomial of degree} \\ N=n-(\ell+1)}} e^{-\rho}\, Y_{\ell m}(\theta,\phi)\,, \end{aligned} \tag{2.34}$$

where $\mathcal{N}$ is a normalization constant. Therefore, using the expression for ρ and absorbing constants into $\mathcal{N}$ we have

$$\boxed{\psi_{n\ell m}(r,\theta,\phi) \;=\; \mathcal{N} \left(\frac{r}{a_0}\right)^{\ell} \begin{pmatrix} \text{polynomial in } \frac{r}{a_0} \\ \text{of degree } N=n-(\ell+1) \end{pmatrix} e^{-\frac{Zr}{na_0}}\, Y_{\ell m}(\theta,\phi)\,.} \tag{2.35}$$

For the ground state of hydrogen ($Z = 1$), we have $(n, \ell, m) = (1, 0, 0)$. Having zero angular momentum the associated wavefunction has no angular dependence. The normalized wavefunction is

$$\psi_{100}(r,\theta\,,\phi) \;=\; \frac{1}{\sqrt{\pi a_0^3}}\, e^{-r/a_0}\,. \tag{2.36}$$

For normalized hydrogen wavefunctions at $n = 2$ and $n = 3$ see
http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hydwf.html

Sarah Geller and Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.